1 Introduction

This paper documents the release of the ELKI data mining framework, version 0.7.5. ELKI is an open source (AGPLv3) data mining software written in Java. The focus of ELKI is research in algorithms, with an emphasis on unsupervised methods in cluster analysis and outlier detection. In order to achieve high performance and scalability, ELKI offers data index structures such as the $\text{RT}^*$-tree that can provide major performance gains. ELKI is designed to be easy to extend for researchers and students in this domain, and welcomes contributions of additional methods. ELKI aims at providing a large collection of highly parameterizable algorithms, in order to allow easy and fair evaluation and benchmarking of algorithms.

We will first outline the motivation for this release, the plans for the future, and then give a brief overview over the new functionality in this version. We also include an appendix presenting an overview on the overall implemented functionality.

2 ELKI 0.7.5: “Heidelberg”

The majority of the work in this release was done at Heidelberg University, both by students (that for example contributed many unit tests as part of Java programming practicals) and by Dr. Erich Schubert. The last official release 0.7.1 is now three years old. Some changes in Java have broken this old release, and it does not run on Java 11 anymore (trivial fixes are long available, but there has not been a released version) – three years where we have continued to add functionality, improve APIs, fix bugs, … yet surprisingly many users still use the old version rather than building the latest development version from git (albeit conveniently available at Github, [https://github.com/elki-project/elki](https://github.com/elki-project/elki)).

There are a number of breaking changes queued up, waiting for a good moment to be pushed. This includes an overhaul of the package names, migration to Java 11, support for automatic indexing, some automatic memory management for automatically added indexes, etc.

Release 0.7.5 is intended as a snapshot to make all the new functionality of the last three years easily available to everybody, and to open a new window where breaking changes are allowed to get in, for the next version 0.8.0.

3 ELKI Plans for the Future

ELKI is an ongoing project. But because of new career responsibilities, the former lead authors will likely be able to devote only much less time to this project in the future.

If you want this project to continue being the largest open-source collection of clustering and outlier detection algorithms – and (not the least because of the support for data indexing) also one of the fastest – then you should consider contributing to this project yourself: for example, by adding missing algorithms from the literature to our collection, fixing smaller bugs, adding completely new functionality, and improving documentation. Thank you.
4 New Functionality in ELKI 0.7.5

4.1 Clustering

• Gaussian Mixture Modeling Improvements:
  ◦ Additional models ◦ Improved numerical stability \(SG18b\) ◦ MAP for robustness ◦ Better initialization
• DBSCAN Improvements:
  ◦ GDBSCAN with similarity functions \(EKSX96\) ◦ Parallel Generalized DBSCAN related to \(PPA^+12\)
• Hierarchical clustering additions:
  ◦ NN-Chain algorithm \(Mur83\) \(Mu11\)
  ◦ MiniMax clustering \(AYN^+05\) \(BT11\)
  ◦ Flexible Beta Linkage \(LW67\)
  ◦ Minimum Variance Linkage \(DLPT85\) \(Pod89\)
• Cluster extraction from dendrograms with handling of noise points and minimum cluster size \(SSW^+17\)
• Basic BIRCH: clustering into leaves, with support for: \(ZRL97\) \(ZRL96\)
• Distances: ◦ Average Intercluster Distance ◦ Average Intracluster Distance ◦ Centroid Euclidean Distance
  ◦ Centroid Manhattan Distance ◦ Variance Increase Distance
• Merge Criteria: ◦ Diameter Criterion ◦ Euclidean Distance Criterion ◦ Radius Criterion
• PAM clustering additions:
  ◦ Reynolds’ PAM \(RRd1RS06\) and FastPAM \(SR18\)
  ◦ Improvements to CLARA \(KR86\) \(KR90a\) and FastCLARA \(SR18\)
  ◦ CLARANS \(NH02\) and FastCLARANS \(SR18\)
• \(k\)-Means clustering additions:
  ◦ Annulus algorithm \(HD14\) \(Dra13\)
  ◦ Exponent algorithm \(NF16\)
  ◦ Simplified Elkan’s algorithm \(NF16\)
  ◦ \(k\)-Means-\(v\) (more robust to noise) \(CG13\)
• \(k\)-Means and PAM initialization additions:
  ◦ Linear Approximative BUILD (LAB) \(SR18\)
  ◦ Ostrovsky’s initial means \(ORSS06\) \(ORSS12\)
  ◦ Park’s initial medoids \(PJ09\)
  ◦ Generated from a normal distribution \(Jan66\)
• Leader Clustering \(Har75\)
• FastDOC subspace clustering \(PJAM02\)

4.2 Association Rule Mining

• Association Rule Generation \(Z14\)
• Interestingness Measures: ◦ Added Value \(SM99\) ◦ Certainty Factor \(GBSM02\) ◦ Confidence \(ALS93\)
  ◦ Conviction \(BMUT97\) ◦ Cosine \(FK00\) ◦ Gini Index \(TK06\) \(RFOS84\) ◦ J Measure \(SG91\) ◦ Jaccard \(vK79\) \(IK04\) ◦ Klosgen \(K96\) ◦ Leverage \(PS91\) ◦ Lift \(BMS97\)

4.3 Outlier Detection

• Cluster-Based Local Outlier Factor (CBLOF) \(HXS03\)
• KNN Data Descriptor (KNND) \(RTD98\)
• Stochastic Outlier Selection (SOS) \(SG17\) \(HPvdH12\), with kNN approximation (KNNSOS) \(SG17\) \(HPvdH12\), and intrinsic dimensionality (ISOS) \(SG17\)

4.4 Projections and Embeddings

• Stochastic Neighbor Embedding (SNE) \(HR02\)
• t-Stochastic Neighbor Embedding (t-SNE) \(vdMH08\)
• Barnes Hut approximation for tSNE \(vdM14\)
• Intrinsic t-SNE \(SG17\)
4.5 Change Point Detection in Time Series

- Offline Change Point Detection [Pg57, BN93, Pic85]
- Signi-Trend-based Change Detection [SWK14]

4.6 Distance and Similarity Functions

- Cosine distances optimized for unit-length vectors • Mahalanobis [Mah36] • Chi Distance [LS03, PRTB99]
- Fisher Rao Distance [DD09, Rao45] • Triangular Discrimination [Top00] • Triangular Distance [CCVR16]

4.7 Evaluation

- Density-Based Cluster Validation (DBCV) [MJC++14]
- Discounted Cumulative Gain (DCG) [JK02]
- Normalized Discounted Cumulative Gain (NDCG) [JK02]

4.8 Indexing Additions

- Basic index support for similarities
- NN Descent [DCL11]
- M-Tree enhancements:
  - Farthest Points Split • MST Split [TTF00] • Balanced Distribution [CPZ97] • Farthest Balanced Distribution
  - Generalized Hyperplane Distribution [CPZ97]
- X-Tree [BKK96] (non-reviewed code)

4.9 Statistics Layer

- Exp-Gamma distribution parameters using the method of moments
- Log-Gamma distribution parameters using the method of moments
- ALID estimator of intrinsic dimensionality [CHK16]

4.10 Other Improvements

- ELKI Builder API (see Section 5)
- Integer range parameters (e.g., 1, 2, ..., 10, 20, ..., 100, 200, ..., 1000)
- Xoroshiro 128 fast random generator [Lem16, BV16]
- Dendrogram visualization for hierarchical clusterings
- Numerous unit tests
- Many bug fixes found in testing and reported by users
5 ELKI Builder API

The ELKI Builder API is a simpler API to initialize classes from Java.
It is based on the standard “builder” pattern, and as it builds upon the Parameterization API, it has support for default values (a feature unfortunately not in the Java API, nor are named parameters).
You can use standard Java constructors, but you will have to specify all parameters:

```java
new KMeansSort<>
    (/* distance= */ EuclideanDistanceFunction.STATIC,
     /* k= */ 10, /* maxiter= */ 0,
     /* init= */ new KMeansPlusPlusInitialMeans<NumberVector>(
         new RandomFactory(/* seed= */ 0L)));
```

For more complex classes such as the R*-tree this can become quite complicated.
If we want to add R-tree indexes (with sort-tile-recursive bulk loading), we can initialize the factory much easier with the ELKIBuilder API, and only specify the page size and bulk load:

```java
new ELKIBuilder<>(RStarTreeFactory.class)
    .with(AbstractPageFileFactory.Parameterizer.PAGE_SIZE_ID, 300)
    .with(RStarTreeFactory.Parameterizer.BULK_SPLIT_ID, SortTileRecursiveBulkSplit.class)
    .build();
```

Furthermore, the parameters directly correspond to the settings in the MiniGUI, hence make it easier to first experiment in the MiniGUI, then transfer these settings into Java code. While in the ELKI unit tests we always use the constants (to enable automatic refactoring), you can also use string parameters here:

```java
new ELKIBuilder<>(RStarTreeFactory.class)
    .with("pagefile.pagesize", 300)
    .with("spatial.bulkstrategy", "str")
    .build();
```

6 Availability

ELKI Release 0.7.5 will be available

- on the project website: [https://elki-project.github.io/releases/](https://elki-project.github.io/releases/)
- on Github: [https://github.com/elki-project/elki/releases](https://github.com/elki-project/elki/releases)
- on Maven central: in the group `de.lmu.ifi.dbs.elki` (0.7.5 will be the last version using this group id)
- via Jitpack: [https://jitpack.io/p/elki-project/elki](https://jitpack.io/p/elki-project/elki) (which also allows accessing development builds)

An example project depending on ELKI is available at [https://github.com/elki-project/example-elki-project](https://github.com/elki-project/example-elki-project)
Appendix

Functionality Available in ELKI 0.7.5

In this Appendix, we give a structured overview of the functionality implemented in ELKI. This is not a complete class list. We only include those classes that are modular, i.e., that can be substituted with other components to configure the data analysis.

Where the classes are annotated with scientific references, we include them in this list, as well as the version when this functionality was introduced in ELKI (possibly with a different name). Note that a reference does not imply this is based on the original code, nor a complete implementation of each paper; but the references can be used to study the underlying ideas of the implementations.

This Appendix is, to a large extend, automatically generated from the ELKI JavaDoc documentation.

Table of Contents

A Algorithm
A.1 Benchmark .............................................. 7
A.2 Classification ......................................... 8
A.3 Clustering ............................................... 8
A.4 Itemsetmining ........................................... 27
A.5 Outlier .................................................. 30
A.6 Projection .............................................. 39
A.7 Statistics ............................................... 40
A.8 Timeseries .............................................. 41

B Application
B.1 Cache .................................................. 42
B.2 Experiments ............................................. 42
B.3 Greedyensemble ........................................ 43

C Data
C.1 Projection ............................................... 44
C.2 Uncertain ............................................... 45

D Database
D.1 Ids ....................................................... 46

E Datasource
E.1 Filter ................................................... 47
E.2 Parser ................................................... 53

F Distance
F.1 Distancefunction ....................................... 55
F.2 Similarityfunction ..................................... 68

G Evaluation
G.1 Classification ......................................... 70
G.2 Clustering .............................................. 70
G.3 Outlier .................................................. 73
G.4 Scores .................................................. 74
A Algorithm

de.lmu.ifi.dbs.elki.algorithm package:
Algorithms suitable as a task for the KDDTask main routine.
The KDDTask main routine expects an algorithm to implement the Algorithm-Interface. Basic functions are already provided within AbstractAlgorithm, see there for basic instructions of how to implement an algorithm suitable to the framework.

Dependency Derivator: Deriving numerical inter-dependencies on data [ABK+06b] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.DependencyDerivator
Dependency derivator computes quantitatively linear dependencies among attributes of a given dataset based on a linear correlation PCA.

KNN-Distance-Order [EKSX96, SSE+17] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.KNNDistancesSampler
Provides an order of the kNN-distances for all objects within the database.
This class can be used to estimate parameters for other algorithms, such as estimating the epsilon parameter for DBSCAN: set k to minPts-1, and then choose a percentile from the sample as epsilon, or plot the result as a graph and look for a bend or knee in this plot.

K-Nearest Neighbor Join (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.KNNJoin
Joins in a given spatial database to each object its k-nearest neighbors. This algorithm only supports spatial databases based on a spatial index structure.
Since this method compares the MBR of every single leaf with every other leaf, it is essentially quadratic in the number of leaves, which may not be appropriate for large trees. It does currently not yet use the tree structure for pruning.

A.1 Benchmark

de.lmu.ifi.dbs.elki.algorithm.benchmark package:
Benchmarking pseudo algorithms.
The algorithms in this package are meant to be used in run time benchmarks, to evaluate e.g. the performance of an index structure.

KNN Benchmark Algorithm (since 0.5.5)
de.lmu.ifi.dbs.elki.algorithm.benchmark.KNNBenchmarkAlgorithm
Benchmarking algorithm that computes the k nearest neighbors for each query point. The query points can either come from a separate data source, or from the original database.

Range Query Benchmark Algorithm (since 0.5.5)
de.lmu.ifi.dbs.elki.algorithm.benchmark.RangeQueryBenchmarkAlgorithm
Benchmarking algorithm that computes a range query for each point. The query points can either come from a separate data source, or from the original database. In the latter case, the database is expected to have an additional, 1-dimensional vector field. For the separate data source, the last dimension will be cut off and used as query radius.
The simplest data setup clearly is to have an input file:
```
x y z label
1 2 3 Example1
4 5 6 Example2
7 8 9 Example3
```
and a query file:
where the additional column is the radius.

Alternatively, if you work with a single file, you need to use the filter command `-dbc.filter Split-NumberVectorFilter -split.dims 1,2,3` to split the relation into a 3-dimensional data vector, and 1 dimensional radius vector.

**Validate Approximative KNN Index**  
*since 0.6.0*  
de.lmu.ifi.dbs.elki.algorithm.benchmark.ValidateApproximativeKNNIndex  
Algorithm to validate the quality of an approximative kNN index, by performing a number of queries and comparing them to the results obtained by exact indexing (e.g. linear scanning).

### A.2 Classification

de.lmu.ifi.dbs.elki.algorithm.classification package:  
Classification algorithms.

**kNN-classifier**  
*since 0.7.0*  
de.lmu.ifi.dbs.elki.algorithm.classification.KNNClassifier  
KNNClassifier classifies instances based on the class distribution among the k nearest neighbors in a database.

**Prior Probability Classifier**  
*since 0.7.0*  
de.lmu.ifi.dbs.elki.algorithm.classification.PriorProbabilityClassifier  
Classifier to classify instances based on the prior probability of classes in the database, without using the actual data values.

### A.3 Clustering

de.lmu.ifi.dbs.elki.algorithm.clustering package:  
Clustering algorithms.

Clustering algorithms are supposed to implement the Algorithm-Interface. The more specialized interface ClusteringAlgorithm requires an implementing algorithm to provide a special result class suitable as a partitioning of the database. More relaxed clustering algorithms are allowed to provide a result that is a fuzzy clustering, does not partition the database complete or is in any other sense a relaxed clustering result.

**Canopy Pre Clustering**  
*MNU00* (since 0.6.0)  
de.lmu.ifi.dbs.elki.algorithm.clustering.CanopyPreClustering  
Canopy pre-clustering is a simple preprocessing step for clustering.

**DBSCAN: Density-Based Clustering of Applications with Noise**  
*EKSX96, SSE+17* (since 0.1)  
de.lmu.ifi.dbs.elki.algorithm.clustering.DBSCAN  
Density-Based Clustering of Applications with Noise (DBSCAN), an algorithm to find density-connected sets in a database.

**GridDBSCAN: Using Grid for Accelerating Density-Based Clustering**  
*MNU08* (since 0.7.1)  
de.lmu.ifi.dbs.elki.algorithm.clustering.GridDBSCAN  
Using Grid for Accelerating Density-Based Clustering.
An accelerated DBSCAN version for numerical data and Lp-norms only, by partitioning the data set into overlapping grid cells. For best efficiency, the overlap of the grid cells must be chosen well. The authors suggest a grid width of 10 times epsilon. Because of partitioning the data, this version does not make use of indexes.

**Leader**

de.lmu.ifi.dbs.elki.algorithm.clustering.Leader

Leader clustering algorithm.

**Naive Mean Shift Clustering**

de.lmu.ifi.dbs.elki.algorithm.clustering.NaiveMeanShiftClustering

Mean-shift based clustering algorithm. Naive implementation: there does not seem to be "the" mean-shift clustering algorithm, but it is a general concept. For the naive implementation, mean-shift is applied to all objects until they converge to other. This implementation is quite naive, and various optimizations can be made.

It also is not really parameter-free: the kernel needs to be specified, including a radius/bandwidth. By using range queries, the algorithm does benefit from index structures!

**SNN: Shared Nearest Neighbor Clustering**

de.lmu.ifi.dbs.elki.algorithm.clustering.SNNClustering

Shared nearest neighbor clustering.

**A.3.1 Affinitypropagation**

de.lmu.ifi.dbs.elki.algorithm.clustering.affinitypropagation

Affinity Propagation (AP) clustering.

**Affinity Propagation: Clustering by Passing Messages Between Data Points**

de.lmu.ifi.dbs.elki.algorithm.clustering.affinitypropagation.AffinityPropagationClusteringAlgorithm

Cluster analysis by affinity propagation.

**Distance Based Initialization With Median**

de.lmu.ifi.dbs.elki.algorithm.clustering.affinitypropagation.DistanceBasedInitializationWithMedian

Distance based initialization.

**Similarity Based Initialization With Median**

de.lmu.ifi.dbs.elki.algorithm.clustering.affinitypropagation.SimilarityBasedInitializationWithMedian

Similarity based initialization.

**A.3.2 Biclustering**

de.lmu.ifi.dbs.elki.algorithm.clustering.biclustering

Biclustering algorithms.

**Cheng And Church**

de.lmu.ifi.dbs.elki.algorithm.clustering.biclustering.CengAndChurch

Cheng and Church biclustering.
A.3.3 Correlation

de.lmu.ifi.dbs.elki.algorithm.clustering.correlation package: Correlation clustering algorithms

**CASH: Robust clustering in arbitrarily oriented subspaces** [ABD*08] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.clustering.correlation.CASH
The CASH algorithm is a subspace clustering algorithm based on the Hough transform.

**COPAC: COrrelation PArtition Clustering** [ABK*07c] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.clustering.correlation.COPAC
COPAC is an algorithm to partition a database according to the correlation dimension of its objects and to then perform an arbitrary clustering algorithm over the partitions.

**ERiC: Exploring Relationships among Correlation Clusters** [ABK*07b] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.clustering.correlation.ERiC
Performs correlation clustering on the data partitioned according to local correlation dimensionality and builds a hierarchy of correlation clusters that allows multiple inheritance from the clustering result.

**4C: Computing Correlation Connected Clusters** [BKKZ04] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.clustering.correlation.FourC
4C identifies local subgroups of data objects sharing a uniform correlation. The algorithm is based on a combination of PCA and density-based clustering (DBSCAN).

**Mining Hierarchies of Correlation Clusters** [ABKZ06] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.clustering.correlation.HiCO
Implementation of the HiCO algorithm, an algorithm for detecting hierarchies of correlation clusters.

**LMCLUS** [HH07] (since 0.5.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.correlation.LMCLUS
Linear manifold clustering in high dimensional spaces by stochastic search.

**ORCLUS: Arbitrarily ORiented projected CLUSter generation** [AY00] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.clustering.correlation.ORCLUS
ORCLUS: Arbitrarily ORiented projected CLUSter generation.

A.3.4 EM

de.lmu.ifi.dbs.elki.algorithm.clustering.em package: Expectation-Maximization clustering algorithm.

**Diagonal Gaussian Model Factory** (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.em.DiagonalGaussianModelFactory
Factory for EM with multivariate gaussian models using diagonal matrices. These models have individual variances, but no covariance, so this corresponds to the 'VVI' model in Mclust (R).

**EM-Clustering: Clustering by Expectation Maximization** [FR07, DLR77] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.clustering.em.EM
Clustering by expectation maximization (EM-Algorithm), also known as Gaussian Mixture Modeling (GMM), with optional MAP regularization.
Multivariate Gaussian Model Factory (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.em.MultivariateGaussianModelFactory
Factory for EM with multivariate Gaussian models (with covariance; also known as Gaussian Mixture Modeling, GMM).
These models have individual covariance matrices, so this corresponds to the 'VVV' model in Mclust (R).

Spherical Gaussian Model Factory (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.em.SphericalGaussianModelFactory
Factory for EM with multivariate gaussian models using a single variance.
These models have a single variances, no covariance, so this corresponds to the 'VII' model in Mclust (R).

Textbook Multivariate Gaussian Model Factory (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.em.TextbookMultivariateGaussianModelFactory
Factory for EM with multivariate Gaussian model, using the textbook algorithm. There is no reason to use this in practice, it is only useful to study the reliability of the textbook approach.
"Textbook" refers to the E[XY]-E[X]E[Y] equation for covariance, that is numerically not reliable with floating point math, but popular in textbooks.
Again, do not use this. Always prefer #MultivariateGaussianModelFactory.

Two Pass Multivariate Gaussian Model Factory (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.em.TwoPassMultivariateGaussianModelFactory
Factory for EM with multivariate Gaussian models (with covariance; also known as Gaussian Mixture Modeling, GMM).
These models have individual covariance matrixes, so this corresponds to the 'VVV' model in Mclust (R).

A.3.5 GDBSCAN
de.lmu.ifi.dbs.elki.algorithm.clustering.gdbscan package:
Generalized DBSCAN. Generalized DBSCAN is an abstraction of the original DBSCAN idea, that allows the use of arbitrary "neighborhood" and "core point" predicates.
For each object, the neighborhood as defined by the "neighborhood" predicate is retrieved - in original DBSCAN, this is the objects within an epsilon sphere around the query object. Then the core point predicate is evaluated to decide if the object is considered dense. If so, a cluster is started (or extended) to include the neighbors as well.

COPAC Neighbor Predicate [ABK+07c] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.gdbscan.COPACNeighborPredicate
COPAC neighborhood predicate.

ERiC Neighbor Predicate [ABK+07b] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.gdbscan.ERiCNeighborPredicate
ERiC neighborhood predicate.

Epsilon Neighbor Predicate [EKSX96] (since 0.5.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.gdbscan.EpsilonNeighborPredicate
The default DBSCAN and OPTICS neighbor predicate, using an epsilon-neighborhood.

Four C Core Predicate [BKKZ04] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.gdbscan.FourCCorePredicate
The 4C core point predicate.
Four C Neighbor Predicate  

4C identifies local subgroups of data objects sharing a uniform correlation. The algorithm is based on a combination of PCA and density-based clustering (DBSCAN).

Generalized DBSCAN  

Generalized DBSCAN, density-based clustering with noise.

LSDBC: Locally Scaled Density Based Clustering  

Locally Scaled Density Based Clustering. This is a variant of DBSCAN which starts with the most dense point first, then expands clusters until density has dropped below a threshold.

MinPts Core Predicate  

The DBSCAN default core point predicate – having at least \( \text{minpts} \) neighbors.

PreDeCon Core Predicate  

The PreDeCon core point predicate – having at least \( \text{minpts} \) neighbors, and a maximum preference dimensionality of lambda.

PreDeCon Neighbor Predicate  

Neighborhood predicate used by PreDeCon.

Similarity Neighbor Predicate  

The DBSCAN neighbor predicate for a \( \text{SimilarityFunction} \), using all neighbors with a minimum similarity.

Gdbscan Parallel  

Parallel versions of Generalized DBSCAN.

Parallel Generalized DBSCAN  

Parallel version of DBSCAN clustering.

A.3.6 Hierarchical  

Hierarchical agglomerative clustering (HAC).
AGNES \[Cor71, KR90b, Sne57\] (since 0.6.0)

delmu.ifi.dbs.elki.algorithm.clustering.hierarchial.AGNES

Hierarchical Agglomerative Clustering (HAC) or Agglomerative Nesting (AGNES) is a classic hierarchical clustering algorithm. Initially, each element is its own cluster; the closest clusters are merged at every step, until all the data has become a single cluster.

This is the naive $O(n^3)$ algorithm. See SLINK for a much faster algorithm (however, only for single-linkage).

This implementation uses the pointer-based representation used by SLINK, so that the extraction algorithms we have can be used with either of them.

The algorithm is believed to be first published (for single-linkage) by:

P. H. Sneath

The application of computers to taxonomy

Journal of general microbiology, 17(1).

This algorithm is also known as AGNES (Agglomerative Nesting), where the use of alternative linkage criterions is discussed:

L. Kaufman, P. J. Rousseeuw

Agglomerative Nesting (Program AGNES),
in Finding Groups in Data: An Introduction to Cluster Analysis

Abstract HDBSCAN \[CMS13\] (since 0.7.0)

delmu.ifi.dbs.elki.algorithm.clustering.hierarchial.AbstractHDBSCAN

Abstract base class for HDBSCAN variations.

Anderberg Hierarchical Clustering \[And73a\] (since 0.7.0)

delmu.ifi.dbs.elki.algorithm.clustering.hierarchial.AnderbergHierarchicalClustering

This is a modification of the classic AGNES algorithm for hierarchical clustering using a nearest-neighbor heuristic for acceleration.

Instead of scanning the matrix (with cost $O(n^3)$) to find the minimum, the nearest neighbor of each object is remembered. On the downside, we need to check these values at every merge, and it may now cost $O(n^3)$ to perform a merge, so there is no worst-case advantage to this approach. The average case however improves from $O(n^3)$ to $O(n^3)$, which yields a considerable improvement in running time.

This optimization is attributed to M. R. Anderberg.

CLINK \[Def77\] (since 0.7.0)

delmu.ifi.dbs.elki.algorithm.clustering.hierarchial.CLINK

CLINK algorithm for complete linkage.

This algorithm runs in $O(n^2)$ time, and needs only $O(n)$ memory. The results can differ from the standard algorithm in unfavorable ways, and are order-dependent (Defays: "Modifications of the labeling permit us to obtain different minimal superior ultrametric dissimilarities"). Unfortunately, the results are usually perceived to be substantially worse than the more expensive algorithms for complete linkage clustering. This arises from the fact that this algorithm has to add the new object to the existing tree in every step, instead of being able to always do the globally best merge.

HDBSCAN: Hierarchical Density-Based Spatial Clustering of Applications with Noise \[CMS13\] (since 0.7.0)

delmu.ifi.dbs.elki.algorithm.clustering.hierarchial.HDBSCANLinearMemory

Linear memory implementation of HDBSCAN clustering.

By not building a distance matrix, we can reduce memory usage to linear memory only; but at the cost of roughly double the runtime (unless using indexes) as we first need to compute all kNN distances (for core sizes), then recompute distances when building the spanning tree.

This implementation follows the HDBSCAN publication more closely than SLINKHDBSCAN, by computing the minimum spanning tree using Prim's algorithm (instead of SLINK; although the two are remarkably similar). In order to produce the preferred internal format of hierarchical clusterings (the compact pointer representation introduced in SLINK) we have to perform a postprocessing conversion.
This implementation does not include the cluster extraction discussed as Step 4, which is provided in a separate step. For this reason, we also do not include self-edges.

**Mini Max**

deb.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.MiniMax

Minimax Linkage clustering.

**Mini Max Anderberg**

deb.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.MiniMaxAnderberg

This is a modification of the classic MiniMax algorithm for hierarchical clustering using a nearest-neighbor heuristic for acceleration.

This particular implementation is based on AnderbergHierarchicalClustering

**Mini Max NN Chain**

deb.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.MiniMaxNNChain

MiniMax hierarchical clustering using the NNchain algorithm.

**SLINK: Single Link Clustering**

deb.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.SLINK

Implementation of the efficient Single-Link Algorithm SLINK of R. Sibson.

This is probably the fastest exact single-link algorithm currently in use.

**SLINKHDBSCAN Linear Memory**

deb.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.SLINKHDBSCANLinearMemory

Linear memory implementation of HDBSCAN clustering based on SLINK.

By not building a distance matrix, we can reduce memory usage to linear memory only; but at the cost of roughly double the runtime (unless using indexes) as we first need to compute all kNN distances (for core sizes), then recompute distances when building the spanning tree.

This version uses the SLINK algorithm to directly produce the pointer representation expected by the extraction methods. The SLINK algorithm is closely related to Prim’s minimum spanning tree, but produces the more compact pointer representation instead of an edges list.

This implementation does not include the cluster extraction discussed as Step 4. This functionality should however already be provided by HDBSCANHierarchyExtraction. For this reason, we also do not include self-edges.

**Hierarchical Birch**

deb.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch package:

BIRCH clustering.

**Average Intercluster Distance**

deb.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch.AverageInterclusterDistance

Average intercluster distance.

**Average Intracluster Distance**

deb.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch.AverageIntraclusterDistance

Average intracluster distance.
BIRCH Leaf Clustering \[ZRL97, ZRL96\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch.BIRCHLeafClustering
BIRCH-based clustering algorithm that simply treats the leaves of the CFTree as clusters.

CF Tree \[ZRL97, ZRL96\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch.CFTree
Partial implementation of the CFTree as used by BIRCH.

Important differences:
1. Leaf nodes and directory nodes have the same capacity
2. Condensing and memory limits are not implemented
3. Merging refinement (merge-resplit) is not implemented

Because we want to be able to track the cluster assignments of all data points easily, we need to store the point IDs, and it is not possible to implement the originally proposed page size management at the same time.

Condensing and merging refinement are possible, and improvements to this code are welcome - please send a pull request!

Centroid Euclidean Distance \[Zha96\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch.CentroidEuclideanDistance
Centroid Euclidean distance.

Centroid Manhattan Distance \[Zha96\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch.CentroidManhattanDistance
Centroid Manhattan Distance

Diameter Criterion \[ZRL96\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch.DiameterCriterion
Average Radius (R) criterion.

Euclidean Distance Criterion (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch.EuclideanDistanceCriterion
Distance criterion.
This is not found in the original work, but used in many implementation attempts: assign points if the Euclidean distances is below a threshold.

Radius Criterion \[ZRL96\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch.RadiusCriterion
Average Radius (R) criterion.

Variance Increase Distance \[Zha96\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.birch.VarianceIncreaseDistance
Variance increase distance.

Hierarchical Extraction de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.extraction package:
Extraction of partitional clusterings from hierarchical results.

Clusters With Noise Extraction \[SSW17\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.extraction.ClustersWithNoiseExtraction
Extraction of a given number of clusters with a minimum size, and noise.
This will execute the highest-most cut where we retain k clusters, each with a minimum size, plus noise (single points that would only merge afterwards). If no such cut can be found, it returns a result with a relaxed k.

You need to specify: A) the minimum size of a cluster (it does not make much sense to use 1 - then it will simply execute all but the last k merges) and B) the desired number of clusters with at least minSize elements each.

Cut Dendrogram By Height
\[ \text{de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.extraction.CutDendrogramByHeight} \]
Extract a flat clustering from a full hierarchy, represented in pointer form.

Cut Dendrogram By Number Of Clusters
\[ \text{de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.extraction.CutDendrogramByNumberOfClusters} \]
Extract a flat clustering from a full hierarchy, represented in pointer form.

HDBSCAN Hierarchy Extraction
\[ \text{de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.extraction.HDBSCANHierarchy} \]
Extraction of simplified cluster hierarchies, as proposed in HDBSCAN.
In contrast to the authors top-down approach, we use a bottom-up approach based on the more efficient pointer representation introduced in SLINK.
In particular, it can also be used to extract a hierarchy from a hierarchical agglomerative clustering.

Simplified Hierarchy Extraction
\[ \text{de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.extraction.SimplifiedHierarchy} \]
Extraction of simplified cluster hierarchies, as proposed in HDBSCAN.
In contrast to the authors top-down approach, we use a bottom-up approach based on the more efficient pointer representation introduced in SLINK.

Hierarchical Linkage
\[ \text{de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.linkage} \]
package:
Linkages for hierarchical clustering.

Centroid Linkage
\[ \text{de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.linkage.CentroidLinkage} \]
Centroid linkage — Unweighted Pair-Group Method using Centroids (UPGMC).
This is closely related to GroupAverageLinkage (UPGMA), but the resulting distance corresponds to the distance of the cluster centroids when used with squared Euclidean distance.
For Lance-Williams, we can then obtain the following recursive definition:
\[ d_{\text{UPGMC}}(A \cup B, C) = \frac{|A|}{|A|+|B|} d(A, C) + \frac{|B|}{|A|+|B|} d(B, C) - \frac{|A||B|}{(|A|+|B|)^2} d(A, B) \]
With squared Euclidean distance, we then get the cluster distance:
\[ d_{\text{UPGMC}}(A, B) = \left\| \frac{1}{|A|} \sum_{a \in A} a - \frac{1}{|B|} \sum_{b \in B} b \right\|^2 \]
but for other distances, this will not generally be true.
Because the ELKI implementations use Lance-Williams, this linkage should only be used with (squared) Euclidean distance.
While titled “unweighted”, this method does take cluster sizes into account when merging clusters with Lance-Williams.
While the idea of this method — at least for squared Euclidean — is compelling (distance of cluster centers), it is not as well behaved as one may think. It can yield so called "inversions", where a later merge has a smaller distance than an early merge, because a cluster center can be closer to a neighboring cluster than any of the individual points. Because of this, the GroupAverageLinkage (UPGMA) is usually preferable.
**Complete Linkage**  
Complete-linkage ("maximum linkage") clustering method.  
The distance of two clusters is simply the maximum of all pairwise distances between the two clusters.  
The distance of two clusters is defined as:

\[
d_{\text{max}}(A, B) := \max_{a \in A} \max_{b \in B} d(a, b)
\]

This can be computed recursively using:

\[
d_{\text{max}}(A \cup B, C) = \max(d(A, C), d(B, C))
\]

Note that with similarity functions, one would need to use the minimum instead to get the same effect.  
The algorithm CLINK is a faster algorithm to find such clusterings, but it is very much order dependent and tends to find worse solutions.

**Flexible Beta Linkage**  
Flexible-beta linkage as proposed by Lance and Williams.  
Beta values larger than 0 cause chaining, and are thus not recommended. Instead, choose a value between -1 and 0.  
The general form of the recursive definition is:

\[
d_{\text{Flexible}, \beta}(A \cup B, C) := \left(1 - \frac{\beta}{2}\right) d(A, C) + \left(1 - \frac{\beta}{2}\right) d(B, C) + \beta d(A, B)
\]

**Group Average Linkage**  
Group-average linkage clustering method (UPGMA).  
This is a good default linkage to use with hierarchical clustering, as it neither exhibits the single-link chaining effect, nor has the strong tendency of complete linkage to split large clusters. It is also easy to understand, and it can be used with arbitrary distances and similarity functions.  
The distances of two clusters is defined as the between-group average distance of two points \(a\) and \(b\), one from each cluster. It should be noted that this is not the average distance within the resulting cluster, because it does not take within-cluster distances into account.  
The distance of two clusters in this method is:

\[
d_{\text{UPGMA}}(A, B) = \frac{1}{|A| \cdot |B|} \sum_{a \in A} \sum_{b \in B} d(a, b)
\]

For Lance-Williams, we can then obtain the following recursive definition:

\[
d_{\text{UPGMA}}(A \cup B, C) = \frac{|A|}{|A| + |B|} d(A, C) + \frac{|B|}{|A| + |B|} d(B, C)
\]

While the method is also called "Unweighted Pair Group Method with Arithmetic mean", it uses weights in the Lance-Williams formulation that account for the cluster size. It is unweighted in the sense that every point keeps the same weight, whereas in WeightedAverageLinkage (WPGMA), the weight of points effectively depends on the depth in the cluster tree.

**Linkage**  
Abstract interface for implementing a new linkage method into hierarchical clustering.

**Median Linkage**  
Median-linkage — weighted pair group method using centroids (WPGMC).  
Similar to WeightedAverageLinkage (WPGMA), the weight of points in this method decreases with the depth of the tree. This yields to difficult to understand semantics of the result, as it does not yield the distance of medians. The method is best defined recursively:

\[
d_{\text{WPGMC}}(A \cup B, C) := \frac{1}{4} d(A, C) + \frac{1}{2} d(B, C) - \frac{1}{4} d(A, B)
\]
**Minimum Variance Linkage** \cite{DLP85, Pod89} (since 0.7.5)

de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.linkage.MinimumVarianceLinkage

Minimum increase in variance (MIVAR) linkage.

This is subtly different from Ward's method (WardLinkage, MISSQ), because variance is normalized by the cluster size; and Ward minimizes the increase in sum of squares (without normalization).

\[
d_{\text{MIVAR}}(A \cup B, C) = \left( \frac{|A|+|C|}{|A|+|B|+|C|} \right)^2 d(A, C) + \left( \frac{|B|+|C|}{|A|+|B|+|C|} \right)^2 d(B, C) - \frac{|C|(|A|+|B|)}{(|A|+|B|+|C|)^2} d(A, B)
\]

or equivalently:

\[
d_{\text{MIVAR}}(A \cup B, C) = \left( \frac{|A|+|C|}{|A|+|B|+|C|} \right)^2 d(A, C) + \left( \frac{|B|+|C|}{|A|+|B|+|C|} \right)^2 d(B, C) - \frac{|C|(|A|+|B|)}{(|A|+|B|+|C|)^2} d(A, B)
\]

**Single Linkage** \cite{FLP+51} (since 0.6.0)

de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.linkage.SingleLinkage

Single-linkage ('minimum') clustering method.

The distance of two clusters is simply the minimum of all pairwise distances between the two clusters.

The distance of two clusters is defined as:

\[
d_{\text{min}}(A, B) := \min_{a \in A} \min_{b \in B} d(a, b)
\]

This can be computed recursively using:

\[
d_{\text{min}}(A \cup B, C) = \min(d(A, C), d(B, C))
\]

Note that with similarity functions, one would need to use the maximum instead to get the same effect.

**Ward Linkage** \cite{Wis69, War63} (since 0.6.0)

de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.linkage.WardLinkage

Ward's method clustering method.

This criterion minimizes the increase of squared errors, and should be used with squared Euclidean distance. Usually, ELKI will try to automatically square distances when you combine this with Euclidean distance.

For performance reasons, the direct use of squared distances is preferable!

The distance of two clusters in this method is:

\[
d_{\text{Ward}}(A, B) := \text{SSE}(A \cup B) - \text{SSE}(A) - \text{SSE}(B)
\]

where the sum of squared errors is defined as:

\[
\text{SSE}(X) := \sum_{x \in X} (x - \mu_X)^2 \quad \text{with} \quad \mu_X = \frac{1}{|X|} \sum_{x \in X} X
\]

This objective can be rewritten to

\[
d_{\text{Ward}}(A, B) := \frac{|A||B|}{|A|+|B|} ||\mu_A - \mu_B||^2 = \frac{1}{|A|+|B|} ||\mu_A - \mu_B||^2
\]

For Lance-Williams, we can then obtain the following recursive definition:

\[
d_{\text{Ward}}(A \cup B, C) = \frac{|A|+|C|}{|A|+|B|+|C|} d(A, C) + \frac{|B|+|C|}{|A|+|B|+|C|} d(B, C) - \frac{|C|}{|A|+|B|+|C|} d(A, B)
\]

These transformations rely on properties of the L2-norm, so they cannot be used with arbitrary metrics, unless they are equivalent to the L2-norm in some transformed space.

Because the resulting distances are squared, when used with a non-squared distance, ELKI implementations will apply the square root before returning the final result. This is statistically somewhat questionable, but usually yields more interpretable distances that — roughly — correspond to the increase in standard deviation. With ELKI, you can get both behavior: Either choose squared Euclidean distance, or regular Euclidean distance.

This method is also referred to as "minimize increase of sum of squares" (MISSQ) by Podani.

**Weighted Average Linkage** \cite{SM02} (since 0.6.0)

de.lmu.ifi.dbs.elki.algorithm.clustering.hierarchical.linkage.WeightedAverageLinkage

Weighted average linkage clustering method (WPGMA).

This is somewhat a misnomer, as it actually ignores that the clusters should likely be weighted differently according to their size when computing the average linkage. See GroupAverageLinkage for the UPGMA.
method that uses the group size to weight the objects the same way. Because of this, it is sometimes also called "simple average".

There does not appear to be a closed form distance for this clustering, but it is only defined recursively on the previous clusters simply by

\[ d_{\text{WPGMA}}(A \cup B, C) := \frac{1}{2}d(A, C) + \frac{1}{2}d(B, C) \]

MedianLinkage (WPGMC) is similar in the sense that it is ignoring the cluster sizes, and therefore the weight of points decreases with the depth of the tree. The method is "weighted" in the sense that the new members get the weight adjusted to match the old cluster members.

A.3.7 Kmeans

de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans package:
K-means clustering and variations.

Best Of Multiple K Means (since 0.6.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.BestOfMultipleKMeans
Run K-Means multiple times, and keep the best run.

CLARA [KR90a, KR86] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.CLARA
Clustering Large Applications (CLARA) is a clustering method for large data sets based on PAM, partitioning around medoids (KMedoidsPAM) based on sampling.

CLARANS [NH02] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.CLARANS
CLARANS: a method for clustering objects for spatial data mining is inspired by PAM (partitioning around medoids, KMedoidsPAM) and CLARA and also based on sampling.
This implementation tries to balance memory and computation time. By caching the distances to the two nearest medoids, we usually only need O(n) instead of O(nk) distance computations for one iteration, at the cost of needing O(2n) memory to store them.
The implementation is fairly ugly, because we have three solutions (the best found so far, the current solution, and a neighbor candidate); and for each point in each solution we need the best and second best assignments. But with Java 11, we may be able to switch to value types that would clean this code significantly, without the overhead of O(n) objects.

Fast CLARA [SR18] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.FastCLARA
Clustering Large Applications (CLARA) with the KMedoidsFastPAM improvements, to increase scalability in the number of clusters. This variant will also default to twice the sample size, to improve quality.

Fast CLARANS [SR18] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.FastCLARANS
A faster variation of CLARANS, that can explore O(k) as many swaps at a similar cost by considering all medoids for each candidate non-medoid. Since this means sampling fewer non-medoids, we suggest to increase the subsampling rate slightly to get higher quality than CLARANS, at better runtime.

K Means Annulus [HD14, Dra13] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansAnnulus
Annulus k-means algorithm. A variant of Hamerly with an additional bound, based on comparing the norm of the mean and the norm of the points.
This implementation could be further improved by precomputing and storing the norms of all points (at the cost of O(n) memory additionally).
K Means Bisecting  
SKK00 (since 0.6.0)  
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansBisecting  
The bisecting k-means algorithm works by starting with an initial partitioning into two clusters, then repeated splitting of the largest cluster to get additional clusters.

Compare-Means  
Phi02 (since 0.7.1)  
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansCompare  
Compare-Means: Accelerated k-means by exploiting the triangle inequality and pairwise distances of means to prune candidate means.

K Means Elkan  
Elk03 (since 0.7.0)  
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansElkan  
Elkan’s fast k-means by exploiting the triangle inequality.  
This variant needs O(n*k) additional memory to store bounds.  
See KMeansHamerly for a close variant that only uses O(n^2) additional memory for bounds.

K Means Exponion  
NF16 (since 0.7.5)  
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansExponion  
Newling's exponion k-means algorithm, exploiting the triangle inequality.  
This is not a complete implementation, the approximative sorting part is missing. We also had to guess on the paper how to make best use of F.

K Means Hamerly  
Ham10 (since 0.7.0)  
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansHamerly  
Hamerly's fast k-means by exploiting the triangle inequality.

k-Means (Lloyd/forgy Algorithm)  
For65 Llo82 (since 0.5.0)  
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansLloyd  
The standard k-means algorithm, using bulk iterations and commonly attributed to Lloyd and Forgy (independently).

k-Means (MacQueen Algorithm)  
Mac67 (since 0.1)  
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansMacQueen  
The original k-means algorithm, using MacQueen style incremental updates; making this effectively an "online" (streaming) algorithm.  
This implementation will by default iterate over the data set until convergence, although MacQueen likely only meant to do a single pass over the data, but the result quality improves with multiple passes.

K-Means-  
CG13 (since 0.7.5)  
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansMinusMinus  
k-means- : A Unified Approach to Clustering and Outlier Detection.  
Similar to Lloyds K-means algorithm, but ignores the farthest points when updating the means, considering them to be outliers.

K Means Simplified Elkan  
NF16 (since 0.7.5)  
de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansSimplifiedElkan  
Simplified version of Elkan’s k-means by exploiting the triangle inequality.  
Compared to KMeansElkan, this uses less pruning, but also does not need to maintain a matrix of pairwise centroid separation.
Sort-Means
\texttt{de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMeansSort} \cite{Phi02} (since 0.7.1)

Sort-Means: Accelerated k-means by exploiting the triangle inequality and pairwise distances of means to prune candidate means (with sorting).

K Medians Lloyd
\texttt{de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMediansLloyd} \cite{BMS96} (since 0.5.0)

k-medians clustering algorithm, but using Lloyd-style bulk iterations instead of the more complicated approach suggested by Kaufman and Rousseeuw (see \texttt{KMedoidsPAM} instead).

K Medoids Fast PAM
\texttt{de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMedoidsFastPAM} \cite{SR18} (since 0.7.5)

FastPAM: An improved version of PAM, that is usually O(k) times faster. This class incorporates the benefits of \texttt{KMedoidsFastPAM1}, but in addition it tries to perform multiple swaps in each iteration (FastPAM2), which can reduce the total number of iterations needed substantially for large k, if some areas of the data are largely independent.

There is a tolerance parameter, which controls how many additional swaps are performed. When set to 0, it will only execute an additional swap if it appears to be independent (i.e., the improvements resulting from the swap have not decreased when the first swap was executed). We suggest to rather leave it at the default of 1, which means to perform any additional swap that gives an improvement. We could not observe a tendency to find worse results when doing these additional swaps, but a reduced runtime.

Because of the speed benefits, we also suggest to use a linear-time initialization, such as the k-means++ initialization or the proposed LAB (linear approximative BUILD, the third component of FastPAM) initialization, and try multiple times if the runtime permits.

K Medoids Fast PAM1
\texttt{de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMedoidsFastPAM1} \cite{SR18} (since 0.7.5)

FastPAM1: A version of PAM that is O(k) times faster, i.e., now in O((n-k)^2). The change here feels pretty small - we handle all k medoids in parallel using an array. But this means the innermost loop only gets executed in O(1/k) of all iterations, and thus we benefit on average.

This acceleration gives exactly (assuming perfect numerical accuracy) the same results as the original PAM. For further improvements that can affect the result, see also \texttt{KMedoidsFastPAM}, which is recommended for usage in practice.

Partitioning Around Medoids
\texttt{de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMedoidsPAM} \cite{KR87,KR90c} (since 0.5.0)

The original Partitioning Around Medoids (PAM) algorithm or k-medoids clustering, as proposed by Kaufman and Rousseeuw in "Clustering by means of Medoids".

K Medoids PAM Reynolds
\texttt{de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMedoidsPAMReynolds} \cite{RRdlIRS06} (since 0.7.5)

The Partitioning Around Medoids (PAM) algorithm with some additional optimizations proposed by Reynolds et al.

In our implementation, we could not observe a substantial improvement over the original PAM algorithm. This may be because of modern CPU architectures, where saving an addition may be negligible compared to caching and pipelining.

K Medoids Park
\texttt{de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.KMedoidsPark} \cite{RRdlIRS06,PJ09} (since 0.5.0)

A k-medoids clustering algorithm, implemented as EM-style bulk algorithm.

In contrast to PAM, which will in each iteration update one medoid with one (arbitrary) non-medoid, this implementation follows the EM pattern. In the expectation step, the best medoid from the cluster members is chosen; in the M-step, the objects are reassigned to their nearest medoid.
This implementation evolved naturally from EM and k-means algorithms, but apparently a similar approach was published by Park and Jun, and also Reynolds et al. discussed this kind of approach before as a side note.

In our experiments, it tends to be much faster than PAM, but also find less good solutions, as the medoids are only chosen from the cluster members. This aligns with findings of Reynolds et al. and can be explained with the requirement of the new medoid to cover the entire cluster.

**Single Assignment K Means** *(since 0.7.0)*

```
<package>de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.SingleAssignmentKMeans</package>
```

Pseudo-k-Means variations, that assigns each object to the nearest center.

**X Means** *(since 0.7.0)*

```
<package>de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.XMeans</package>
```

X-means: Extending K-means with Efficient Estimation on the Number of Clusters.

Note: this implementation does currently not use a k-d-tree for acceleration. Also note that kmax is not a hard threshold - the algorithm can return up to 2^kmax clusters!

**Kmeans Initialization**

```
<package>de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.initialization</package>
```

Initialization strategies for k-means.

- **Farthest Points Initial Means** *(since 0.6.0)*

```
<package>de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.initialization.FarthestPointsInitialMeans</package>
```

K-Means initialization by repeatedly choosing the farthest point (by the minimum distance to earlier points).

Note: this is less random than other initializations, so running multiple times will be more likely to return the same local minima.

- **Farthest Sum Points Initial Means** *(since 0.6.0)*

```
<package>de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.initialization.FarthestSumPointsInitialMeans</package>
```

K-Means initialization by repeatedly choosing the farthest point (by the sum of distances to previous objects).

Note: this is less random than other initializations, so running multiple times will be more likely to return the same local minima.

- **First K Initial Means** *(since 0.5.0)*

```
<package>de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.initialization.FirstKInitialMeans</package>
```

Initialize K-means by using the first k objects as initial means.

- **K Means Plus Plus Initial Means** *(since 0.5.0)*

```
<package>de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.initialization.KMeansPlusPlusInitialMeans</package>
```

K-Means++ initialization for k-means.

- **LAB Initial Means** *(since 0.7.5)*

```
<package>de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.initialization.LABInitialMeans</package>
```

Linear approximative BUILD (LAB) initialization for FastPAM (and k-means).

This is a O(nk) approximation of the original PAM BUILD. For performance, it uses an O(sqrt(n)) sample to achieve linear run time. The results will be worse than those of BUILD, but provide a good starting point for FastPAM optimization.
Ostrovsky Initial Means

Ostrovsky initial means, a variant of k-means++ that is expected to give slightly better results on average, but only works for k-means and not for, e.g., PAM (k-medoids).

PAM Initial Means

PAM initialization for k-means (and of course, for PAM).

Park Initial Means

Initialization method proposed by Park and Jun.

It is easy to imagine that this approach can become problematic, because it does not take the distances between medoids into account. In the worst case, it may choose k duplicates as initial centers, therefore we cannot recommend this strategy, but it is provided for completeness.

Predefined Initial Means

Run k-means with prespecified initial means.

Random Normal Generated Initial Means

Initialize k-means by generating random vectors (normal distributed with $N(\mu, \sigma)$ in each dimension).

This is a different interpretation of the work of Jancey, who wrote little more details but "introduced into known but arbitrary positions"; but seemingly worked with standardized scores. In contrast to RandomUniformGeneratedInitialMeans (which uses a uniform on the entire value range), this class uses a normal distribution based on the estimated parameters. The resulting means should be more central, and thus a bit less likely to become empty (at least if you assume there is no correlation amongst attributes...it is still not competitive with better methods).

Warning: this still tends to produce empty clusters in many situations, and is one of the least effective initialization strategies, not recommended for use.

Random Uniform Generated Initial Means

Initialize k-means by generating random vectors (uniform, within the value range of the data set).

This is attributed to Jancey, but who wrote little more details but "introduced into known but arbitrary positions". This class assumes this refers to uniform positions within the value domain. For a normal distributed variant, see RandomNormalGeneratedInitialMeans.

Warning: this tends to produce empty clusters, and is one of the least effective initialization strategies, not recommended for use.

Randomly Chosen Initial Means

Initialize K-means by randomly choosing k existing elements as initial cluster centers.

Sample K Means Initialization

Initialize k-means by running k-means on a sample of the data set only.
**Kmeans Parallel**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.parallel` package:  
Parallelized implementations of k-means.

**Parallel Lloyd K Means**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.parallel.ParallelLloydKMeans`  
(since 0.7.0)  
Parallel implementation of k-Means clustering.

**Kmeans Quality**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.quality` package:  
Quality measures for k-Means results.

**Abstract K Means Quality Measure**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.quality.AbstractKMeansQualityMeasure`  
Base class for evaluating clusterings by information criteria (such as AIC or BIC). Provides helper functions (e.g. max likelihood calculation) to its subclasses.

**Akaike Information Criterion**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.quality.AkaikeInformationCriterion`  
[PM00, Aka73] (since 0.7.0)  
Akaike Information Criterion (AIC).

**Bayesian Information Criterion**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.quality.BayesianInformationCriterion`  
[Sch78] (since 0.7.0)  
Bayesian Information Criterion (BIC), also known as Schwarz criterion (SBC, SBIC) for the use with evaluating k-means results.

**Bayesian Information Criterion Zhao**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.quality.BayesianInformationCriterionZhao`  
[ZXF08] (since 0.7.0)  
Different version of the BIC criterion.

**Within Cluster Mean Distance Quality Measure**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.quality.WithinClusterMeanDistanceQualityMeasure`  
(since 0.6.0)  
Class for computing the average overall distance.  
The average of all average pairwise distances in a cluster.

**Within Cluster Variance Quality Measure**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.kmeans.quality.WithinClusterVarianceQualityMeasure`  
(since 0.6.0)  
Class for computing the variance in a clustering result (sum-of-squares).

**A.3.8 Meta**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.meta` package:  
Meta clustering algorithms, that get their result from other clusterings or external sources.

**External Clustering**  
`de.lmu.ifi.dbs.elki.algorithm.clustering.meta.ExternalClustering`  
(since 0.7.0)  
Read an external clustering result from a file, such as produced by ClusteringVectorDumper.  
The input format of this parser is text-based:  
```plaintext  
# Optional comment  
1 1 1 2 2 2 -1 Example label  
```  
Where non-negative numbers are cluster assignments, negative numbers are considered noise clusters.
A.3.9 Onedimensional

de.lmu.ifi.dbs.elki.algorithm.clustering.onedimensional package:
Clustering algorithms for one-dimensional data.

KNN Kernel Density Minima Clustering (since 0.6.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.onedimensional.KNNKernelDensityMinimaClustering
Cluster one-dimensional data by splitting the data set on local minima after performing kernel density estimation.

A.3.10 Optics

de.lmu.ifi.dbs.elki.algorithm.clustering.optics package:
OPTICS family of clustering algorithms.
Note that some OPTICS based algorithms (HiCO, DiSH) are in the subspace and correlation packages, which better describes their use case.

Abstract OPTICS [ABKS99] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.optics.AbstractOPTICS
The OPTICS algorithm for density-based hierarchical clustering.
This is the abstract base class, providing the shared parameters only.

DeliClu: Density-Based Hierarchical Clustering [ABK06c] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.clustering.optics.DeliClu
DeliClu: Density-Based Hierarchical Clustering
A hierarchical algorithm to find density-connected sets in a database, closely related to OPTICS but exploiting the structure of a R-tree for acceleration.

Fast OPTICS [SV13] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.optics.FastOPTICS
FastOPTICS algorithm (Fast approximation of OPTICS)
Note that this is not FOPTICS as in "Fuzzy OPTICS!"

OPTICS: Density-Based Hierarchical Clustering (implementation using a heap) [ABKS99] (since 0.1)
de.lmu.ifi.dbs.elki.algorithm.clustering.optics.OPTICSHep
The OPTICS algorithm for density-based hierarchical clustering.
Algorithm to find density-connected sets in a database based on the parameters 'minPts' and 'epsilon' (specifying a volume). These two parameters determine a density threshold for clustering.
This implementation uses a heap.

OPTICS: Density-Based Hierarchical Clustering (implementation using a list) [ABKS99] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.optics.OPTICSList
The OPTICS algorithm for density-based hierarchical clustering.
Algorithm to find density-connected sets in a database based on the parameters 'minPts' and 'epsilon' (specifying a volume). These two parameters determine a density threshold for clustering.
This version is implemented using a list, always scanning the list for the maximum. While this could be cheaper than the complex heap updates, benchmarks indicate the heap version is usually still preferable.

OPTICS Xi Cluster Extraction [ABKS99, SG18a] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.clustering.optics.OPTICSEXi
Extract clusters from OPTICS Plots using the original Xi extraction.
A.3.11 Subspace

de.lmu.ifi.dbs.elki.algorithm.clustering.subspace package:

Axis-parallel subspace clustering algorithms

The clustering algorithms in this package are instances of both, projected clustering algorithms or subspace clustering algorithms according to the classical but somewhat obsolete classification schema of clustering algorithms for axis-parallel subspaces.

CLIQUE: Automatic Subspace Clustering of High Dimensional Data for Data Mining Applications

[AGGR98] (since 0.1)

de.lmu.ifi.dbs.elki.algorithm.clustering.subspace.CLIQUE

Implementation of the CLIQUE algorithm, a grid-based algorithm to identify dense clusters in subspaces of maximum dimensionality.

The implementation consists of two steps:
1. Identification of subspaces that contain clusters
2. Identification of clusters

The third step of the original algorithm (Generation of minimal description for the clusters) is not (yet) implemented.

Note: this is fairly old code, and not well optimized. Do not use this for runtime benchmarking!

DOC: Density-based Optimal projective Clustering

[PJAM02] (since 0.6.0)

de.lmu.ifi.dbs.elki.algorithm.clustering.subspace.DOC

DOC is a sampling based subspace clustering algorithm.

DiSH: Detecting Subspace cluster Hierarchies

[ABK+07a] (since 0.1)

de.lmu.ifi.dbs.elki.algorithm.clustering.subspace.DiSH

Algorithm for detecting subspace hierarchies.

FastDOC: Density-based Optimal projective Clustering

[PJAM02] (since 0.7.5)

de.lmu.ifi.dbs.elki.algorithm.clustering.subspace.FastDOC

The heuristic variant of the DOC algorithm, FastDOC.

Finding Hierarchies of Subspace Clusters

[ABK+06a] (since 0.1)

de.lmu.ifi.dbs.elki.algorithm.clustering.subspace.HiSC

Implementation of the HiSC algorithm, an algorithm for detecting hierarchies of subspace clusters.

P3C: A Robust Projected Clustering Algorithm.

[MSE06] (since 0.6.0)

de.lmu.ifi.dbs.elki.algorithm.clustering.subspace.P3C

P3C: A Robust Projected Clustering Algorithm.

PROCLUS: PROjected CLUStering

[AWY+99] (since 0.1)

de.lmu.ifi.dbs.elki.algorithm.clustering.subspace.PROCLUS

The PROCLUS algorithm, an algorithm to find subspace clusters in high dimensional spaces.

PreDeCon: Subspace Preference weighted Density Connected Clustering

[BKKK04] (since 0.1)

de.lmu.ifi.dbs.elki.algorithm.clustering.subspace.PreDeCon

PreDeCon computes clusters of subspace preference weighted connected points. The algorithm searches for local subgroups of a set of feature vectors having a low variance along one or more (but not all) attributes.
SUBCLU: Density connected Subspace Clustering

Implementation of the SUBCLU algorithm, an algorithm to detect arbitrarily shaped and positioned clusters in subspaces. SUBCLU delivers for each subspace the same clusters DBSCAN would have found, when applied to this subspace separately.

A.3.12 Uncertain

Clustering algorithms for uncertain data.

CK Means

Run k-means on the centers of each uncertain object.

Center Of Mass Meta Clustering

Center-of-mass meta clustering reduces uncertain objects to their center of mass, then runs a vector-oriented clustering algorithm on this data set.

FDBSCAN: Density-based Clustering of Applications with Noise on fuzzy objects

This implementation is based on GeneralizedDBSCAN. All implementation of FDBSCAN functionality is located in the neighbor predicate FDBSCANNeighborPredicate.

FDBSCAN Neighbor Predicate

Density-based Clustering of Applications with Noise and Fuzzy objects (FDBSCAN) is an Algorithm to find sets in a fuzzy database that are density-connected with minimum probability.

Representative Uncertain Clustering

This algorithm clusters uncertain data by repeatedly sampling a possible world, then running a traditional clustering algorithm on this sample.

The resulting "possible" clusterings are then clustered themselves, using a clustering similarity measure. This yields a number of representatives for the set of all possible worlds.

UK Means

Uncertain K-Means clustering, using the average deviation from the center.

Note: this method is, essentially, superficial. It was shown to be equivalent to doing regular K-means on the object centroids instead (see CKMeans for the reference and an implementation). This is only for completeness.

A.4 Itemsetmining

Algorithms for frequent itemset mining such as APRIORI.
**APRIORI: Algorithm for Mining Association Rules**

The APRIORI algorithm for Mining Association Rules.

**Eclat**

Eclat is a depth-first discovery algorithm for mining frequent itemsets.

This implementation is the basic algorithm only, and does not use diffsets. Columns are represented using a sparse representation, which theoretically is beneficial when the density is less than 1/31. This corresponds roughly to a minimum support of 3% for 1-itemsets. When searching for itemsets with a larger minimum support, it may be desirable to use a dense bitset representation instead and/or implement an automatic switching technique!

Performance of this implementation is probably surpassed with a low-level C implementation based on SIMD bitset operations as long as support of an itemset is high, which are not easily accessible in Java.

**FP Growth**

FP-Growth is an algorithm for mining the frequent itemsets by using a compressed representation of the database called FPGrowth.FPTree.

FP-Growth first sorts items by the overall frequency, since having high frequent items appear first in the tree leads to a much smaller tree since frequent subsets will likely share the same path in the tree. FP-Growth is beneficial when you have a lot of (near-) duplicate transactions, and are using a not too high support threshold, as it only prunes single items, not item combinations.

This implementation is in-memory only, and has not yet been carefully optimized.

The worst case memory use probably is $O(\min(n \cdot l, i))$ where $i$ is the number of items, $l$ the average itemset length, and $n$ the number of items. The worst case scenario is when every item is frequent, and every transaction is unique. The resulting tree will then be larger than the original data.

**A.4.1 Association rules**

Association rule mining.

**Association Rule Generation**

This algorithm calls a specified frequent itemset algorithm and calculates all association rules, having an interest value between then the specified boundaries form the obtained frequent itemsets

**Association rules Interest**

Association rule interestingness measures.

Much of the confusion with these measures arises from the anti-monotonicity of itemsets, which are omnipresent in the literature.

In the itemset notation, the itemset $X$ denotes the set of matching transactions $\{T|X \subseteq T\}$ that contain the itemset $X$. If we enlarge $Z = X \cup Y$, the resulting set shrinks: $\{T|Z \subseteq T\} = \{T|X \subseteq T\} \cap \{T|Y \subseteq T\}$. Because of this: $\text{support}(X \cup Y) = P(X \cap Y)$ and $\text{support}(X \cap Y) = P(X \cup Y)$. With "support" and "confidence", it is common to see the reversed semantics (the union on the constraints is the intersection on the matches, and conversely); with probabilities it is common to use "events" as in frequentist inference. To make things worse, the "support" is sometimes in absolute (integer) counts, and sometimes used in a relative share.
Added Value \[SM99\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.AddedValue
Added value (AV) interestingness measure: confidence\(X \rightarrow Y\) – support\(Y\) = \(P(Y|X) - P(Y)\).

Certainty Factor \[GBSM02\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.CertaintyFactor
Certainty factor (CF; Loevinger) interestingness measure. \[
\frac{\text{confidence}(X \rightarrow Y) - \text{support}(Y)}{\text{support}(Y)}.
\]

Confidence \[AIS93\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.Confidence
Confidence interestingness measure, \[
\frac{\text{support}(X \cup Y)}{\text{support}(X)} = \frac{P(X \cap Y)}{P(X)} = P(Y|X).
\]

Conviction \[BMUT97\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.Conviction
Conviction interestingness measure: \[
\frac{P(X)P(Y)}{P(X \cap Y)}.
\]

Cosine \[TK00\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.Cosine
Cosine interestingness measure, \[
\frac{\text{support}(A \cup B)}{\sqrt{\text{support}(A) \cdot \text{support}(B)}} = \frac{P(A \cap B)}{\sqrt{P(A)P(B)}}.
\]
The interestingness measure called IS by Tan and Kumar.

Gini Index \[TK00\] [BFOSS4] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.GiniIndex
Gini-index based interestingness measure, using the weighted squared conditional probabilities compared to the non-conditional priors.
\[
P(X) (P(Y|X)^2 + P(\neg Y|X)^2) + P(\neg X) (P(Y|\neg X)^2 + P(\neg Y|\neg X)^2) - P(Y)^2 - P(\neg Y)^2
\]

J Measure \[SG91\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.JMeasure
J-Measure interestingness measure. \[
P(X \cap Y) \log \frac{P(Y|X)}{P(Y\neg Y)} + P(X \cap \neg Y) \log \frac{P(Y\neg X)}{P(Y\neg Y)}.
\]

Jaccard \[GR79\] [TKS04] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.Jaccard
Jaccard interestingness measure:
\[
\frac{\text{support}(A \cup B)}{\text{support}(A \cap B)} = \frac{P(\neg A \cap \neg B)}{P(\neg A \cap A) + P(\neg B \cap B) - P(\neg A \cap B)} = \frac{P(A \cap B)}{P(A \cup B)}.
\]

Klosgen \[Klo96\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.Klosgen
Klösgen interestingness measure.
\[
\sqrt{\text{support}(X \cup Y) (\text{confidence}(X \rightarrow Y) - \text{support}(Y) = \sqrt{P(X \cap Y) (P(Y|X) - P(Y))}
\]

Leverage \[PS91\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.Leverage
Leverage interestingness measure.
\[
\text{support}(X \Rightarrow Y) - \text{support}(X)\text{support}(Y) = P(X \cap Y) - P(X)P(Y)
\]

Lift \[BMS97\] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.itemsetmining.associationrules.interest.Lift
Lift interestingness measure.
\[
\frac{\text{confidence}(X \rightarrow Y)}{\text{support}(Y)} = \frac{\text{confidence}(Y \rightarrow X)}{\text{support}(X)} = \frac{P(X \cap Y)}{P(X)P(Y)}
\]
A.5 Outlier

Outlier detection algorithms

delmu.ifi.dbs.elki.algorithm.outlier package:

COP: Correlation Outlier Probability

delmu.ifi.dbs.elki.algorithm.outlier.COP
Correlation outlier probability: Outlier Detection in Arbitrarily Oriented Subspaces

DWOF: Dynamic Window Outlier Factor

delmu.ifi.dbs.elki.algorithm.outlier.DWOF
Algorithm to compute dynamic-window outlier factors in a database based on a specified parameter k, which specifies the number of the neighbors to be considered during the calculation of the DWOF score.

Gaussian Model Outlier Detection

delmu.ifi.dbs.elki.algorithm.outlier.GaussianModel
Outlier detection based on the probability density of the single normal distribution.

Gaussian-Uniform Mixture Model Outlier Detection

delmu.ifi.dbs.elki.algorithm.outlier.GaussianUniformMixture
Outlier detection algorithm using a mixture model approach. The data is modeled as a mixture of two distributions, a Gaussian distribution for ordinary data and a uniform distribution for outliers. At first all Objects are in the set of normal objects and the set of anomalous objects is empty. An iterative procedure then transfers objects from the ordinary set to the anomalous set if the transfer increases the overall likelihood of the data.

OPTICS-OF: Identifying Local Outliers

delmu.ifi.dbs.elki.algorithm.outlier.OPTICSOF
OPTICS-OF outlier detection algorithm, an algorithm to find Local Outliers in a database based on ideas from OPTICSTypeAlgorithm clustering.

Simple COP: Correlation Outlier Probability

delmu.ifi.dbs.elki.algorithm.outlier.SimpleCOP
Algorithm to compute local correlation outlier probability. This is the simpler, original version of COP, as published in

A.5.1 Anglebased

Angle-based outlier detection algorithms.

ABOD: Angle-Based Outlier Detection

delmu.ifi.dbs.elki.algorithm.outlier.anglebased.ABOD
Angle-Based Outlier Detection / Angle-Based Outlier Factor. Outlier detection using variance analysis on angles, especially for high dimensional data sets. Exact version, which has cubic runtime (see also FastABOD and LBABOD for faster versions).

Approximate ABOD: Angle-Based Outlier Detection

delmu.ifi.dbs.elki.algorithm.outlier.anglebased.FastABOD
Fast-ABOD (approximateABOF) version of Angle-Based Outlier Detection / Angle-Based Outlier Factor. Note: the minimum k is 3. The 2 nearest neighbors yields one 1 angle, which implies a constant 0 variance everywhere.
LB-ABOD: Lower Bounded Angle-Based Outlier Detection

de.lmu.ifi.dbs.elki.algorithm.outlier.anglebased.LBABOD

LB-ABOD (lower-bound) version of Angle-Based Outlier Detection / Angle-Based Outlier Factor.

Outlier detection using variance analysis on angles, especially for high dimensional data sets.

A.5.2 Clustering

de.lmu.ifi.dbs.elki.algorithm.outlier.clustering package:

Clustering based outlier detection.

Discovering cluster-based local outliers

de.lmu.ifi.dbs.elki.algorithm.outlier.clustering.CBLOF

Cluster-based local outlier factor (CBLOF).

EM Outlier: Outlier Detection based on the generic EM clustering

de.lmu.ifi.dbs.elki.algorithm.outlier.clustering.EMOutlier

Outlier detection algorithm using EM Clustering.

If an object does not belong to any cluster it is supposed to be an outlier. If the probability for an object to
belong to the most probable cluster is still relatively low this object is an outlier.

K Means Outlier Detection

de.lmu.ifi.dbs.elki.algorithm.outlier.clustering.KMeansOutlierDetection

Outlier detection by using k-means clustering.

The scores are assigned by the objects distance to the nearest center.

We don’t have a clear reference for this approach, but it seems to be a best practise in some areas to remove
objects that have the largest distance from their center. If you need to cite this approach, please cite the
ELKI version you used (use the ELKI publication list for citation information and BibTeX templates).

Silhouette Outlier Detection

de.lmu.ifi.dbs.elki.algorithm.outlier.clustering.SilhouetteOutlierDetection

Outlier detection by using the Silhouette Coefficients.

Silhouette values are computed as by Rousseeuw and then used as outlier scores. To cite this outlier
detection approach, please cite the ELKI version you used (use the ELKI publication list for citation
information and BibTeX templates).

A.5.3 Distance

de.lmu.ifi.dbs.elki.algorithm.outlier.distance package:

Distance-based outlier detection algorithms, such as DBOutlier and kNN.

For methods based on local density, see package de.lmu.ifi.dbs.elki.algorithm.outlier.lof instead.

Abstract DB Outlier

de.lmu.ifi.dbs.elki.algorithm.outlier.distance.AbstractDBOutlier

Simple distance based outlier detection algorithms.

DBOD: Distance Based Outlier Detection

de.lmu.ifi.dbs.elki.algorithm.outlier.distance.DBOutlierDetection

Simple distance-based outlier detection algorithm. User has to specify two parameters An object is flagged
as an outlier if at least a fraction p of all data objects has a distance above d from c.
Distance Based Outlier Score
\cite{KN98} (since 0.3)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.DBOutlierScore
Compute percentage of neighbors in the given neighborhood with size $d$.
Generalization of the DB Outlier Detection by using the fraction as outlier score thus eliminating this parameter and turning the method into a ranking method instead of a labelling one.

Fast Outlier Detection in High Dimensional Spaces
\cite{AP02} (since 0.5.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.HilOut
Fast Outlier Detection in High Dimensional Spaces
Outlier Detection using Hilbert space filling curves

KNNDD: k-Nearest Neighbor Data Description
\cite{dRTD98} (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.KNNDD
Nearest Neighbor Data Description.
A variation inbetween of KNN outlier and LOF, comparing the nearest neighbor distance of a point to the nearest neighbor distance of the nearest neighbor.
The initial description used $k=1$, where this equation makes most sense. For $k > 1$, one may want to use averaging similar to LOF.

KNN outlier: Efficient Algorithms for Mining Outliers from Large Data Sets
\cite{RRS00} (since 0.3)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.KNNOutlier
Outlier Detection based on the distance of an object to its $k$ nearest neighbor.
This implementation differs from the original pseudocode: the $k$ nearest neighbors do not exclude the point that is currently evaluated. I.e. for $k=1$ the resulting score is the distance to the 1-nearest neighbor that is not the query point and therefore should match $k=2$ in the exact pseudocode - a value of $k=1$ in the original code does not make sense, as the 1NN distance will be 0 for every point in the database. If you for any reason want to use the original algorithm, subtract 1 from the $k$ parameter.

KNNSOS: k-Nearest-Neighbor Stochastic Outlier Selection
\cite{SG17, JHPvdH12} (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.KNNSOS
kNN-based adaption of Stochastic Outlier Selection.
This is a trivial variation of Stochastic Outlier Selection to benefit from KNN indexes, but not discussed in the original publication. Instead of setting perplexity, we choose the number of neighbors $k$, and set perplexity simply to $k/3$. Objects outside of the kNN are not considered anymore.

KNNWeight outlier detection
\cite{AP02} (since 0.3)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.KNNWeightOutlier
Outlier Detection based on the accumulated distances of a point to its $k$ nearest neighbors.
As in the original publication (as far as we could tell from the pseudocode included), the current point is not included in the nearest neighbors (see figures in the publication). This matches the intuition common in nearest neighbor classification, where the evaluated instances are not part of the training set; but it contrasts to the pseudocode of the kNN outlier method and the database interpretation (which returns all objects stored in the database).
Furthermore, we report the sum of the $k$ distances (called "weight" in the original publication). Other implementations may return the average distance instead, and therefore yield different results.

Local Isolation Coefficient
\cite{YSW09} (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.LocalIsolationCoefficient
The Local Isolation Coefficient is the sum of the kNN distance and the average distance to its $k$ nearest neighbors.
The algorithm originally used a normalized Manhattan distance on numerical attributes, and Hamming distance on categorical attributes.
ODIN: Outlier Detection Using k-Nearest Neighbour Graph [HKF04] (since 0.6.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.ODIN
Outlier detection based on the in-degree of the kNN graph.
This is a curried version: instead of using a threshold T to obtain a binary decision, we use the computed value as outlier score; normalized by k to make the numbers more comparable across different parameterizations.

An Efficient Reference-based Approach to Outlier Detection in Large Datasets [PZG06] (since 0.3)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.ReferenceBasedOutlierDetection
Reference-Based Outlier Detection algorithm, an algorithm that computes kNN distances approximately, using reference points.
kNN distances are approximated by the difference in distance from a reference point. For this approximation to be of high quality, triangle inequality is required; but the algorithm can also process non-metric distances.

SOS: Stochastic Outlier Selection [SG17, JHPvdH12] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.SOS
Stochastic Outlier Selection.

Distance Parallel de.lmu.ifi.dbs.elki.algorithm.outlier.distance.parallel package:
Parallel implementations of distance-based outlier detectors.

Parallel KNN Outlier [SZK14b] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.parallel.ParallelKNNOutlier
Parallel implementation of KNN Outlier detection.

Parallel KNN Weight Outlier [SZK14b] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.distance.parallel.ParallelKNNWeightOutlier
Parallel implementation of KNN Weight Outlier detection.

A.5.4 Intrinsic
de.lmu.ifi.dbs.elki.algorithm.outlier.intrinsic package:
Outlier detection algorithms based on intrinsic dimensionality.

IDOS: Intrinsic Dimensional Outlier Score [vBHZ15] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.intrinsic.IDOS
Intrinsic Dimensional Outlier Detection in High-Dimensional Data.

ISOS: Intrinsic Stochastic Outlier Selection [SG17] (since 0.7.5)
de.lmu.ifi.dbs.elki.algorithm.outlier.intrinsic.ISOS
Intrinsic Stochastic Outlier Selection.

Intrinsic Dimensionality Outlier [HSZ18] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.intrinsic.IntrinsicDimensionalityOutlier
Use intrinsic dimensionality for outlier detection.

A.5.5 Lof
de.lmu.ifi.dbs.elki.algorithm.outlier.lof package:
LOF family of outlier detection algorithms.
Approximate LOCI: Fast Outlier Detection Using the Local Correlation Integral  
\[\text{de.lmu.ifi.dbs.elki.algorithm.outlier.lof.ALOCI}\]  
Fast Outlier Detection Using the "approximate Local Correlation Integral".  
Outlier detection using multiple epsilon neighborhoods.

COF: Connectivity-based Outlier Factor  
\[\text{de.lmu.ifi.dbs.elki.algorithm.outlier.lof.COF}\]  
Connectivity-based Outlier Factor (COF).

FlexibleLOF: Local Outlier Factor with additional options  
\[\text{de.lmu.ifi.dbs.elki.algorithm.outlier.lof.FlexibleLOF}\]  
Flexible variant of the "Local Outlier Factor" algorithm.  
This implementation diverts from the original LOF publication in that it allows the user to use a different  
distance function for the reachability distance and neighborhood determination (although the default is to  
use the same value.)  
The k nearest neighbors are determined using the standard distance function, while the reference set used  
in reachability distance computation is configured using a separate reachability distance function.  
The original LOF parameter was called "minPts". For consistency with the name "kNN query", we chose  
to rename the parameter to k. Flexible LOF allows you to set the two values different, which yields the  
parameters \(-\text{lof.krefer}\) and \(-\text{lof.kreach}\).

INFLO: Influenced Outlierness Factor  
\[\text{de.lmu.ifi.dbs.elki.algorithm.outlier.lof.INFLO}\]  
Influence Outliers using Symmetric Relationship (INFLO) using two-way search, is an outlier detection  
method based on LOF; but also using the reverse kNN.

KDEOS: Kernel Density Estimator Outlier Score  
\[\text{de.lmu.ifi.dbs.elki.algorithm.outlier.lof.KDEOS}\]  
Generalized Outlier Detection with Flexible Kernel Density Estimates.  
This is an outlier detection inspired by LOF, but using kernel density estimation (KDE) from statistics.  
Unfortunately, for higher dimensional data, kernel density estimation itself becomes difficult. At this point,  
the kdeos.idim parameter can become useful, which allows to either disable dimensionality adjustment  
completely (0) or to set it to a lower dimensionality than the data representation. This may sound like  
a hack at first, but real data is often of lower intrinsic dimensionality, and embedded into a higher data  
representation. Adjusting the kernel to account for the representation seems to yield worse results than  
using a lower, intrinsic, dimensionality.  
If your data set has many duplicates, the kdeos.kernel.minbw parameter sets a minimum kernel band-  
width, which may improve results in these cases, as it prevents kernels from degenerating to single  
points.

LDF: Outlier Detection with Kernel Density Functions  
\[\text{de.lmu.ifi.dbs.elki.algorithm.outlier.lof.LDF}\]  
Outlier Detection with Kernel Density Functions.  
A variation of LOF which uses kernel density estimation, but in contrast to SimpleKernelDensityLOF  
also uses the reachability concept of LOF.

LDOF: Local Distance-Based Outlier Factor  
\[\text{de.lmu.ifi.dbs.elki.algorithm.outlier.lof.LDOF}\]  
Computes the LDOF (Local Distance-Based Outlier Factor) for all objects of a Database.
LOCI: Fast Outlier Detection Using the Local Correlation Integral

Fast Outlier Detection Using the "Local Correlation Integral".
Exact implementation only, not aLOCI. See ALOCI.
Outlier detection using multiple epsilon neighborhoods.
This implementation has O(n^3 log n) runtime complexity!

LOF: Local Outlier Factor

Algorithm to compute density-based local outlier factors in a database based on a specified parameter -lof.k.
The original LOF parameter was called "minPts", but for consistency within ELKI we have renamed this parameter to "k".
Compatibility note: as of ELKI 0.7.0, we no longer include the query point, for consistency with other methods.

LoOP: Local Outlier Probabilities

Distance/density based algorithm similar to LOF to detect outliers, but with statistical methods to achieve better result stability.

Online LOF

Incremental version of the LOF Algorithm, supports insertions and removals.

Simple Kernel Density LOF

A simple variant of the LOF algorithm, which uses a simple kernel density estimation instead of the local reachability density.

Simplified LOF

A simplified version of the original LOF algorithm, which does not use the reachability distance, yielding less stable results on inliers.

Variance Of Volume

Variance of Volume for outlier detection.
The volume is estimated by the distance to the k-nearest neighbor, then the variance of volume is computed.
Unfortunately, this approach needs an enormous numerical precision, and may not work for high-dimensional, non-normalized data. We therefore divide each volume by the average across the data set. This means values are even less comparable across data sets, but this avoids some of the numerical problems of this method.

Lof Parallel

Parallelized variants of LOF.
This parallelization is based on the generalization of outlier detection published in:

Parallel LOF

Parallel implementation of Local Outlier Factor using processors.
This parallelized implementation is based on the easy-to-parallelize generalized pattern discussed in Erich Schubert, Arthur Zimek, Hans-Peter Kriegel
Local Outlier Detection Reconsidered: a Generalized View on Locality with Applications to Spatial, Video, and Network Outlier Detection
Data Mining and Knowledge Discovery 28(1)

Parallel Simplified LOF [SZK14b] (since 0.7.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.lof.parallel.ParallelSimplifiedLOF
Parallel implementation of Simplified-LOF Outlier detection using processors.

A.5.6 Meta
de.lmu.ifi.dbs.elki.algorithm.outlier.meta package:
Meta outlier detection algorithms: external scores, score rescaling.

External Double Outlier Score (since 0.4.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.meta.ExternalDoubleOutlierScore
External outlier detection scores, loading outlier scores from an external file. This class is meant to be able to read the default output of ELKI, i.e. one object per line, with the DBID specified as ID= and the outlier score specified with an algorithm-specific prefix.

Feature Bagging for Outlier Detection [LK05] (since 0.4.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.meta.FeatureBagging
A simple ensemble method called "Feature bagging" for outlier detection. Since the proposed method is only sensible to run on multiple instances of the same algorithm (due to incompatible score ranges), we do not allow using arbitrary algorithms.

HiCS: High Contrast Subspaces for Density-Based Outlier Ranking [KMB12] (since 0.5.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.meta.HiCS
Algorithm to compute High Contrast Subspaces for Density-Based Outlier Ranking.

Rescale Meta Outlier Algorithm (since 0.4.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.meta.RescaleMetaOutlierAlgorithm
Scale another outlier score using the given scaling function.

Simple Outlier Ensemble (since 0.5.5)
de.lmu.ifi.dbs.elki.algorithm.outlier.meta.SimpleOutlierEnsemble
Simple outlier ensemble method.

A.5.7 Spatial
de.lmu.ifi.dbs.elki.algorithm.outlier.spatial package:
Spatial outlier detection algorithms

GLS-Backward Search [CLR10] (since 0.4.0)
de.lmu.ifi.dbs.elki.algorithm.outlier.spatial.CTLuGLSBackwardSearchAlgorithm
GLS-Backward Search is a statistical approach to detecting spatial outliers.
Implementation note: this is just the most basic version of this algorithm. The spatial relation must be two
dimensional, the set of spatial basis functions is hard-coded (but trivial to enhance) to \(\{1, x, y, x^2, y^2, xy\}\), and
we assume the neighborhood is large enough for the simpler formulas to work that make the optimization
problem convex.

**CTLu Mean Multiple Attributes**

```
CTLuMeanMultipleAttributes
```

Mean Approach is used to discover spatial outliers with multiple attributes.

**Median Algorithm for Spatial Outlier Detection**

```
CTLuMedianAlgorithm
```

Median Algorithm of C.-T. Lu

**CTLu Median Multiple Attributes**

```
CTLuMedianMultipleAttributes
```

Median Approach is used to discover spatial outliers with multiple attributes.

**Moran Scatterplot Outlier**

```
CTLuMoranScatterplotOutlier
```

Moran scatterplot outliers, based on the standardized deviation from the local and global means. In contrast
to the definition given in the reference, we use this as a ranking outlier detection by not applying the
signedness test, but by using the score \((- \text{localZ}) \times \text{Average localZ of Neighborhood}\) directly. This allows
us to differentiate a bit between stronger and weaker outliers.

**Random Walk on Exhaustive Combination**

```
CTLuRandomWalkEC
```

Spatial outlier detection based on random walks.

Note: this method can only handle one-dimensional data, but could probably be easily extended to higher
dimensional data by using an distance function instead of the absolute difference.

**Scatterplot Spatial Outlier**

```
CTLuScatterplotOutlier
```

Scatterplot-outlier is a spatial outlier detection method that performs a linear regression of object attributes
and their neighbors average value.

**Z-Test Outlier Detection**

```
CTLuZTestOutlier
```

Detect outliers by comparing their attribute value to the mean and standard deviation of their neighborhood.

**SLOM: a new measure for local spatial outliers**

```
SLOM
```

SLOM: a new measure for local spatial outliers

**Spatial Outlier Factor**

```
SOF
```

The Spatial Outlier Factor (SOF) is a spatial LOF variation.

Since the “reachability distance” of LOF cannot be used canonically in the bichromatic case, this part of
LOF is dropped and the exact distance is used instead.

**A Trimmed Mean Approach to Finding Spatial Outliers**

```
TrimmedMeanApproach
```

A Trimmed Mean Approach to Finding Spatial Outliers.
Outliers are defined by their value deviation from a trimmed mean of the neighbors.

**Spatial Neighborhood**  
de.lmu.ifi.dbs.elki.algorithm.outlier.spatial.neighborhood package:  
Spatial outlier neighborhood classes

**Extended Neighborhood**  
de.lmu.ifi.dbs.elki.algorithm.outlier.spatial.neighborhood.ExtendedNeighborhood  
Neighborhood obtained by computing the k-fold closure of an existing neighborhood.

**External Neighborhood**  
de.lmu.ifi.dbs.elki.algorithm.outlier.spatial.neighborhood.ExternalNeighborhood  
A precomputed neighborhood, loaded from an external file.

**Precomputed K Nearest Neighbor Neighborhood**  
de.lmu.ifi.dbs.elki.algorithm.outlier.spatial.neighborhood.PrecomputedKNearestNeighbor  
Neighborhoods based on k nearest neighbors.

### A.5.8 Subspace

de.lmu.ifi.dbs.elki.algorithm.outlier.subspace package:
Subspace outlier detection methods.
Methods that detect outliers in subspaces (projections) of the data set.

**Abstract Aggarwal Yu Outlier**  
de.lmu.ifi.dbs.elki.algorithm.outlier.subspace.AbstractAggarwalYuOutlier  
Abstract base class for the sparse-grid-cell based outlier detection of Aggarwal and Yu.

**EA FOD: the evolutionary outlier detection algorithm**  
de.lmu.ifi.dbs.elki.algorithm.outlier.subspace.AggarwalYuEvolutionary  
Evolutionary variant (EAFOD) of the high-dimensional outlier detection algorithm by Aggarwal and Yu.

**BruteForce: Outlier detection for high dimensional data**  
de.lmu.ifi.dbs.elki.algorithm.outlier.subspace.AggarwalYuNaive  
BruteForce variant of the high-dimensional outlier detection algorithm by Aggarwal and Yu.
The evolutionary approach is implemented as AggarwalYuEvolutionary

**OUTRES**  
de.lmu.ifi.dbs.elki.algorithm.outlier.subspace.OUTRES  
Adaptive outlierness for subspace outlier ranking (OUTRES).
Note: this algorithm seems to have a $O(n!d!)$ complexity with no obvious way to accelerate it with usual index structures for range queries: each object in each tested subspace will need to know the mean and standard deviation of the density of the neighbors, which in turn needs another range query; except if we precomputed the densities for each of $O(d!)$ possible subsets of dimensions.

**OutRank: ranking outliers in high dimensional data**  
de.lmu.ifi.dbs.elki.algorithm.outlier.subspace.OutRankS1  
OutRank: ranking outliers in high dimensional data.
Algorithm to score outliers based on a subspace clustering result. This class implements score 1 of the OutRank publication, which is a score based on cluster sizes and cluster dimensionality.
SOD: Subspace outlier degree

Subspace Outlier Degree. Outlier detection method for axis-parallel subspaces.

A.5.9 Svm

Support-Vector-Machines for outlier detection.

LibSVM One Class Outlier Detection

Outlier-detection using one-class support vector machines.

Important note: from literature, the one-class SVM is trained as if 0 was the only counterexample. Outliers will only be detected when they are close to the origin in kernel space! In our experience, results from this method are rather mixed, in particular as you would likely need to tune hyperparameters. Results may be better if you have a training data set with positive examples only, then apply it only to new data (which is currently not supported in this implementation, it assumes a single-dataset scenario).

A.6 Projection

Data projections (see also preprocessing filters for basic projections).

Barnes Hut TSNE

tSNE using Barnes-Hut-Approximation.

For larger data sets, use an index to make finding the nearest neighbors faster, e.g. cover tree or k-d-tree.

Gaussian Affinity Matrix Builder

Compute the affinity matrix for SNE and tSNE using a Gaussian distribution with a constant sigma.

Intrinsic t-Stochastic Neighbor Embedding

Build sparse affinity matrix using the nearest neighbors only, adjusting for intrinsic dimensionality. On data sets with high intrinsic dimensionality, this can give better results.

Furthermore, this approach uses a different rule to combine affinities: rather than taking the arithmetic average of $p_{ij}$ and $p_{ji}$, we use $\sqrt{p_{ij} \cdot p_{ji}}$, which prevents outliers from attaching closely to nearby clusters.

Nearest Neighbor Affinity Matrix Builder

Build sparse affinity matrix using the nearest neighbors only.

Perplexity Affinity Matrix Builder

Compute the affinity matrix for SNE and tSNE.

SNE

Stochastic Neighbor Embedding is a projection technique designed for visualization that tries to preserve the nearest neighbor structure.
t-SNE
[vdMH08] (since 0.7.5)

de.lmu.ifi.dbs.elki.algorithm.projection.TSNE

t-Stochastic Neighbor Embedding is a projection technique designed for visualization that tries to preserve the nearest neighbor structure.

A.7 Statistics

de.lmu.ifi.dbs.elki.algorithm.statistics package:

Statistical analysis algorithms.

The algorithms in this package perform statistical analysis of the data (e.g. compute distributions, distance distributions etc.)

Add Single Scale

de.lmu.ifi.dbs.elki.algorithm.statistics.AddSingleScale (since 0.5.0)

Pseudo "algorithm" that computes the global min/max for a relation across all attributes.

Add Uniform Scale

de.lmu.ifi.dbs.elki.algorithm.statistics.AddUniformScale (since 0.7.5)

Pseudo "algorithm" that computes the global min/max for a relation across all attributes.

Average Precision At K

de.lmu.ifi.dbs.elki.algorithm.statistics.AveragePrecisionAtK (since 0.5.0)

Evaluate a distance functions performance by computing the average precision at k, when ranking the objects by distance.

Distance Quantile Sampler

de.lmu.ifi.dbs.elki.algorithm.statistics.DistanceQuantileSampler (since 0.7.0)

Compute a quantile of a distance sample, useful for choosing parameters for algorithms.

Distance Histogram

de.lmu.ifi.dbs.elki.algorithm.statistics.DistanceStatisticsWithClasses (since 0.2)

Algorithm to gather statistics over the distance distribution in the data set.

Estimate Intrinsic Dimensionality

de.lmu.ifi.dbs.elki.algorithm.statistics.EstimateIntrinsicDimensionality (since 0.7.0)

Estimate global average intrinsic dimensionality of a data set.

Note: this algorithm does not produce a result, but only logs statistics.

Evaluate Ranking Quality

de.lmu.ifi.dbs.elki.algorithm.statistics.EvaluateRankingQuality (since 0.2)

Evaluate a distance function with respect to kNN queries. For each point, the neighbors are sorted by distance, then the ROC AUC is computed. A score of 1 means that the distance function provides a perfect ordering of relevant neighbors first, then irrelevant neighbors. A value of 0.5 can be obtained by random sorting. A value of 0 means the distance function is inverted, i.e. a similarity.

In contrast to RankingQualityHistogram, this method uses a binning based on the centrality of objects. This allows analyzing whether or not a particular distance degrades for the outer parts of a cluster.

Evaluate Retrieval Performance

de.lmu.ifi.dbs.elki.algorithm.statistics.EvaluateRetrievalPerformance (since 0.7.0)

Evaluate a distance functions performance by computing the mean average precision, ROC, and NN classification performance when ranking the objects by distance.
Hopkins Statistic Clustering Tendency

de.lmu.ifi.dbs.elki.algorithm.statistics.HopkinsStatisticClusteringTendency

The Hopkins Statistic of Clustering Tendency measures the probability that a data set is generated by a uniform data distribution.

The statistic compares the ratio of the 1NN distance for objects from the data set compared to the 1NN distances of uniform distributed objects.

Range Query Selectivity

de.lmu.ifi.dbs.elki.algorithm.statistics.RangeQuerySelectivity

Evaluate the range query selectivity.

Ranking Quality Histogram

de.lmu.ifi.dbs.elki.algorithm.statistics.RankingQualityHistogram

Evaluate a distance function with respect to kNN queries. For each point, the neighbors are sorted by distance, then the ROC AUC is computed. A score of 1 means that the distance function provides a perfect ordering of relevant neighbors first, then irrelevant neighbors. A value of 0.5 can be obtained by random sorting. A value of 0 means the distance function is inverted, i.e. a similarity.

A.8 Timeseries

de.lmu.ifi.dbs.elki.algorithm.timeseries package:

Off-line Change Point Detection

de.lmu.ifi.dbs.elki.algorithm.timeseries.OfflineChangePointDetectionAlgorithm

Off-line change point detection algorithm detecting a change in mean, based on the cumulative sum (CUSUM), same-variance assumption, and using bootstrap sampling for significance estimation.

Signi-Trend: scalable detection of emerging topics in textual streams by hashed significance thresholds

de.lmu.ifi.dbs.elki.algorithm.timeseries.SigniTrendChangeDetection

Signi-Trend detection algorithm applies to a single time-series. This is not a complete implementation of the method, but a modified (two-sided) version of the significance score use in Signi-Trend for change detection. The hashing and scalability parts of Signi-Trend are not applicable here.

This implementation currently does not use timestamps, and thus only works for fixed-interval measurements. It could be extended to allow dynamic data windows by adjusting the alpha parameter based on time deltas.

B Application

de.lmu.ifi.dbs.elki.application package:

Abstract Application

de.lmu.ifi.dbs.elki.application.AbstractApplication

AbstractApplication sets the values for flags verbose and help. Any Wrapper class that makes use of these flags may extend this class. Beware to make correct use of parameter settings via optionHandler as commented with constructor and methods.

Classifier Holdout Evaluation Task

de.lmu.ifi.dbs.elki.application.ClassifierHoldoutEvaluationTask

Evaluate a classifier.
**Convert To Bundle Application**  
\texttt{de.lmu.ifi.dbs.elki.application.ConvertToBundleApplication}  
(since 0.5.5)  
Convert an input file to the more efficient ELKI bundle format.

**Generator XML Spec**  
\texttt{de.lmu.ifi.dbs.elki.application.GeneratorXMLSpec}  
(since 0.2)  
Generate a data set based on a specified model (using an XML specification)

**KDDCLI Application**  
\texttt{de.lmu.ifi.dbs.elki.application.KDDCLIApplication}  
(since 0.3)  
Basic command line application for Knowledge Discovery in Databases use cases. It allows running unsupervised Algorithms to run on any DatabaseConnection.

### B.1 Cache

\texttt{de.lmu.ifi.dbs.elki.application.cache} package:  
Utility applications for the persistence layer such as distance cache builders.  
\texttt{CacheDoubleDistanceInOnDiskMatrix} and \texttt{CacheFloatDistanceInOnDiskMatrix} are conversion utilities that materialize an arbitrary distance into a binary distance cache on the harddisk (using OnDiskUpperTriangleMatrix)

**Cache Double Distance In On Disk Matrix**  
\texttt{de.lmu.ifi.dbs.elki.application.cache.CacheDoubleDistanceInOnDiskMatrix}  
(since 0.2)  
Precompute an on-disk distance matrix, using double precision.

**Cache Double Distance KNN Lists**  
\texttt{de.lmu.ifi.dbs.elki.application.cache.CacheDoubleDistanceKNNLists}  
(since 0.6.0)  
Precompute the k nearest neighbors in a disk cache.

**Cache Double Distance Range Queries**  
\texttt{de.lmu.ifi.dbs.elki.application.cache.CacheDoubleDistanceRangeQueries}  
(since 0.6.0)  
Precompute the k nearest neighbors in a disk cache.

**Cache Float Distance In On Disk Matrix**  
\texttt{de.lmu.ifi.dbs.elki.application.cache.CacheFloatDistanceInOnDiskMatrix}  
(since 0.2)  
Precompute an on-disk distance matrix, using float precision.

**Precompute Distances Ascii Application**  
\texttt{de.lmu.ifi.dbs.elki.application.cache.PrecomputeDistancesAsciiApplication}  
(since 0.2)  
Application to precompute pairwise distances into an ascii file.  
IDs in the output file will always begin at 0.  
The result can then be used with the DoubleDistanceParse.  
Symmetry is assumed.

### B.2 Experiments

\texttt{de.lmu.ifi.dbs.elki.application.experiments} package:  
Packaged experiments to make them easy to reproduce.

**Evaluate Intrinsic Dimensionality Estimators**  
\texttt{de.lmu.ifi.dbs.elki.application.experiments.EvaluateIntrinsicDimensionalityEstimators}  
(since 0.7.0)  
Class for testing the estimation quality of intrinsic dimensionality estimators.
Visualize Geodesic Distances
[SZK13] (since 0.5.5)
de.lmu.ifi.dbs.elki.application.experiments.VisualizeGeodesicDistances
Visualization function for Cross-track, Along-track, and minimum distance function.

B.3 Greedyensemble

de.lmu.ifi.dbs.elki.application.greedyensemble package:
Greedy ensembles for outlier detection.
This package contains code used for the greedy ensemble experiment in Erich Schubert, Remigius Wojdanowski, Arthur Zimek, Hans-Peter Kriegel
On Evaluation of Outlier Rankings and Outlier Scores
Proc. 12th SIAM Int. Conf. on Data Mining (SDM 2012)

Compute KNN Outlier Scores
[SWZK12] (since 0.5.0)
de.lmu.ifi.dbs.elki.application.greedyensemble.ComputeKNNOutlierScores
Application that runs a series of kNN-based algorithms on a data set, for building an ensemble in a second step. The output file consists of a label and one score value for each object.
Since some algorithms can be too slow to run on large data sets and for large values of k, they can be disabled. For example -disable (LDOF|DWOF|COF|FastABOD)’ disables these two methods completely. Alternatively, you can use the parameter -ksquaremax to control the maximum k for these four methods separately.
For methods where k=1 does not make sense, this value will be skipped, and the procedure will commence at 1+stepsize.

Evaluate Precomputed Outlier Scores
(since 0.7.0)
de.lmu.ifi.dbs.elki.application.greedyensemble.EvaluatePrecomputedOutlierScores
Class to load an outlier detection summary file, as produced by ComputeKNNOutlierScores, and compute popular evaluation metrics for it.
File format description:
• Each column is one object in the data set
• Each line is a different algorithm
• There is a mandatory label column, containing the method name
• The first line must contain the ground-truth, titled bylabel, where 0 indicates an inlier and 1 indicates an outlier
The evaluation assumes that high scores correspond to outliers, unless the method name matches the pattern given using -reversed. The default value matches several scores known to use reversed values.

Greedy Ensemble Experiment
[SWZK12] (since 0.5.0)
de.lmu.ifi.dbs.elki.application.greedyensemble.GreedyEnsembleExperiment
Class to load an outlier detection summary file, as produced by ComputeKNNOutlierScores, and compute a naive ensemble for it. Based on this initial estimation, and optimized ensemble is built using a greedy strategy. Starting with the best candidate only as initial ensemble, the most diverse candidate is investigated at each step. If it improves towards the (estimated) target vector, it is added, otherwise it is discarded.
This approach is naive, and it may be surprising that it can improve results. The reason is probably that diversity will result in a comparable ensemble, while the reduced ensemble size is actually responsible for the improvements, by being more decisive and less noisy due to dropping ‘unhelpful’ members.
This still leaves quite a bit of room for improvement. If you build upon this basic approach, please acknowledge our proof of concept work.

Visualize Pairwise Gain Matrix
[SWZK12] (since 0.5.0)
de.lmu.ifi.dbs.elki.application.greedyensemble.VisualizePairwiseGainMatrix
Class to load an outlier detection summary file, as produced by ComputeKNNOutlierScores, and compute a matrix with the pairwise gains. It will have one column / row obtained for each combination.
The gain is always computed in relation to the better of the two input methods. Green colors indicate the result has improved, red indicate it became worse.

C  Data

de.lmu.ifi.dbs.elki.data package:
Basic classes for different data types, database object types and label types.

Hierarchical Class Label (since 0.1)
de.lmu.ifi.dbs.elki.data.HierarchicalClassLabel
A HierarchicalClassLabel is a ClassLabel to reflect a hierarchical structure of classes.

Simple Class Label (since 0.1)
de.lmu.ifi.dbs.elki.data.SimpleClassLabel
A simple class label casting a String as it is as label.

C.1  Projection

de.lmu.ifi.dbs.elki.data.projection package:
Data projections.

Feature Selection (since 0.5.0)
de.lmu.ifi.dbs.elki.data.projection.FeatureSelection
Projection class for number vectors.

LatLngToECEF Projection (since 0.6.0)
de.lmu.ifi.dbs.elki.data.projection.LatLngToECEFProjection
Project (Latitude, Longitude) vectors to (X, Y, Z), from spherical coordinates to ECEF (earth-centered earth-fixed).

LngLatToECEF Projection (since 0.6.0)
de.lmu.ifi.dbs.elki.data.projection.LngLatToECEFProjection
Project (Longitude, Latitude) vectors to (X, Y, Z), from spherical coordinates to ECEF (earth-centered earth-fixed).

Numerical Feature Selection (since 0.5.0)
de.lmu.ifi.dbs.elki.data.projection.NumericalFeatureSelection
Projection class for number vectors.

Random Projection (since 0.6.0)
de.lmu.ifi.dbs.elki.data.projection.RandomProjection
Randomized projections of the data.
This class allows projecting the data with different types of random projections, in particular database friendly projections (as suggested by Achlioptas, see AchlioptasRandomProjectionFamily), but also as suggested for locality sensitive hashing (LSH).

C.1.1  Random

de.lmu.ifi.dbs.elki.data.projection.random package:
Random projection families.
Achlioptas Random Projection Family \[\text{[Ach01]}\] (since 0.6.0)
de.lmu.ifi.dbs.elki.data.projection.random.AchlioptasRandomProjectionFamily
Random projections as suggested by Dimitris Achlioptas.

Cauchy Random Projection Family \[\text{[DIIM04]}\] (since 0.6.0)
de.lmu.ifi.dbs.elki.data.projection.random.CauchyRandomProjectionFamily
Random projections using Cauchy distributions (1-stable).

Gaussian Random Projection Family \[\text{[DIIM04]}\] (since 0.6.0)
de.lmu.ifi.dbs.elki.data.projection.random.GaussianRandomProjectionFamily
Random projections using Cauchy distributions (1-stable).

Random Subset Projection Family \[\text{[Bre96]}\] (since 0.6.0)
de.lmu.ifi.dbs.elki.data.projection.random.RandomSubsetProjectionFamily
Random projection family based on selecting random features.
The basic idea of using this for data mining should probably be attributed to L. Breiman, who used it to improve the performance of predictors in an ensemble.

Simplified Random Hyperplane Projection Family \[\text{[Hen06]}\] (since 0.7.0)
de.lmu.ifi.dbs.elki.data.projection.random.SimplifiedRandomHyperplaneProjectionFamily
Random hyperplane projection family.

C.2 Uncertain
de.lmu.ifi.dbs.elki.data.\texttt{uncertain} package:
Uncertain data objects.

Unweighted Discrete Uncertain Object \[\text{[DRS09, BSHW06]}\] (since 0.7.0)
de.lmu.ifi.dbs.elki.data.\texttt{uncertain.UnweightedDiscreteUncertainObject}
Unweighted implementation of discrete uncertain objects.
• Every object is represented by a finite number of discrete samples.
• Every sample has the same weight.
• Every sample is equally likely to be returned by \texttt{drawSample(java.util.Random)}.

Weighted Discrete Uncertain Object \[\text{[DRS09, BSHW06, BKR}^+09\text{]}\] (since 0.7.0)
de.lmu.ifi.dbs.elki.data.\texttt{uncertain.WeightedDiscreteUncertainObject}
Weighted version of discrete uncertain objects.
• Every object is represented by a finite number of discrete samples.
• Every sample has a weight associated with it.
• Samples with higher weight are more likely to be returned by \texttt{drawSample(java.util.Random)}.

C.2.1 Uncertainifier
de.lmu.ifi.dbs.elki.data.\texttt{uncertain.uncertainifier} package:
Classes to generate uncertain objects from existing certain data.

Simple Gaussian Uncertainifier \textcolor{red}{(since 0.7.0)}
de.lmu.ifi.dbs.elki.data.\texttt{uncertain.uncertainifier.SimpleGaussianUncertainifier}
Vector factory

Uniform Uncertainifier \textcolor{red}{(since 0.7.0)}
de.lmu.ifi.dbs.elki.data.\texttt{uncertain.uncertainifier.UniformUncertainifier}
Factory class.
Unweighted Discrete Uncertainifier (since 0.7.0)
de.lmu.ifi.dbs.elki.data.uncertain.uncertainifier.UnweightedDiscreteUncertainifier
Class to generate unweighted discrete uncertain objects.
This is a second-order generator: it requires the use of another generator to sample from (e.g. UniformUncertainifier or SimpleGaussianUncertainifier).

Weighted Discrete Uncertainifier (since 0.7.0)
de.lmu.ifi.dbs.elki.data.uncertain.uncertainifier.WeightedDiscreteUncertainifier
Class to generate weighted discrete uncertain objects.
This is a second-order generator: it requires the use of another generator to sample from (e.g. UniformUncertainifier or SimpleGaussianUncertainifier).

D Database
de.lmu.ifi.dbs.elki.database package:
ELKI database layer - loading, storing, indexing and accessing data

D.1 Ids
de.lmu.ifi.dbs.elki.database.ids package:
Database object identification and ID group handling API.
Database IDs (short: DBID) in ELKI are based on the factory pattern, to allow replacing the simple Integer-based DBIDs with more complex implementations, e.g. for use with external databases or to add tracking for debugging purposes. This also allows adding of more efficient implementations later on in a single place.

DBID interface:
The DBID object identifies a single object.
The DBIDs hierarchy contains classes for handling groups (sets, arrays) of IDs, that can be seen as a two-dimensional matrix consisting

ArrayDBIDs HashSetDBIDs
ModifiableDBIDs ArrayModifiableDBIDs HashSetModifiableDBIDs
StaticDBIDs ArrayStaticDBIDs n/a

StaticDBIDs are structures that cannot support modifications, but thus can be implemented more efficiently, for example as Interval. They are mostly used by the data sources.
These interfaces cannot be instantiated, obviously. Instead, use the static DBIDFactory.FACTORY, which is also wrapped in the DBIDUtil class.

Examples:

`DBIDs allids = database.getIDs();
// preallocate an array of initial capacity 123
ArrayModifiableDBIDs array = DBIDUtil.newArraySet(123);
// new DBID hash set with minimum initial capacity
ModifiableDBIDs hash = DBIDUtil.newHashSet();
// add all DBIDs from the hash
tree.addDBIDs(hash)`

Utility functions:

- `DBIDUtil.ensureArray` to ensure ArrayDBIDs
- `DBIDUtil.ensureModifiable` to ensure ModifiableDBIDs
- `DBIDUtil.makeUnmodifiable` to wrap DBIDs unmodifiable
Generic utility classes:

MaskedDBIDs allows masking an ArrayDBIDs with a BitSet.

D.1.1 Integer

*de.lmu.ifi.dbs.elki.database.ids.integer* package:
Integer-based DBID implementation – do not use directly - always use DBIDUtil.

**Integer DBID Array Quick Sort**  \(^{(Yar09)}\) (since 0.5.5)

*de.lmu.ifi.dbs.elki.database.ids.integer.*IntegerDBIDArrayQuickSort*
Class to sort an integer DBID array, using a modified quicksort.
Two array iterators will be used to seek to the elements to compare, while the backing storage is a plain integer array.

**Reusing DBID Factory**  \((\text{since } 0.4.0)\)

*de.lmu.ifi.dbs.elki.database.ids.integer.*ReusingDBIDFactory*
Slightly more complex DBID management, that allows reuse of DBIDs.
NOT tested a lot yet. Not reusing is much simpler!

**Simple DBID Factory**  \((\text{since } 0.4.0)\)

*de.lmu.ifi.dbs.elki.database.ids.integer.*SimpleDBIDFactory*
Simple DBID management, that never reuses IDs. Statically allocated DBID ranges are given positive values, Dynamically allocated DBIDs are given negative values.

**Trivial DBID Factory**  \((\text{since } 0.4.0)\)

*de.lmu.ifi.dbs.elki.database.ids.integer.*TrivialDBIDFactory*
Trivial DBID management, that never reuses IDs and just gives them out in sequence. All IDs will be positive.

E Datasource

*de.lmu.ifi.dbs.elki.datasource* package:
Data normalization (and reconstitution) of data sets.

E.1 Filter

*de.lmu.ifi.dbs.elki.datasource.filter* package:
Data filtering, in particular for normalization and projection.

**Fixed DBIDs Filter**  \((\text{since } 0.4.0)\)

*de.lmu.ifi.dbs.elki.datasource.filter.*FixedDBIDsFilter*
This filter assigns static DBIDs, based on the sequence the objects appear in the bundle by adding a column of DBID type to the bundle.

E.1.1 Cleaning

*de.lmu.ifi.dbs.elki.datasource.filter.*cleaning* package:
Filters for data cleaning.
Drop Na N Filter
\[ \text{de.lmu.ifi.dbs.elki.datasource.filter.cleaning.DropNaNFilter} \] (since 0.6.0)
A filter to drop all records that contain NaN values.
Note: currently, only dense vector columns are supported.

No Missing Values Filter
\[ \text{de.lmu.ifi.dbs.elki.datasource.filter.cleaning.NoMissingValuesFilter} \] (since 0.4.0)
A filter to remove entries that have missing values.

Replace Na N With Random Filter
\[ \text{de.lmu.ifi.dbs.elki.datasource.filter.cleaning.ReplaceNaNWithRandomFilter} \] (since 0.6.0)
A filter to replace all NaN values with random values.
Note: currently, only dense vector columns are supported.

Vector Dimensionality Filter
\[ \text{de.lmu.ifi.dbs.elki.datasource.filter.cleaning.VectorDimensionalityFilter} \] (since 0.7.0)
Filter to remove all vectors that do not have the desired dimensionality.

E.1.2 Normalization
\[ \text{de.lmu.ifi.dbs.elki.datasource.filter.normalization package:} \]
Data normalization.

Normalization Columnwise
\[ \text{de.lmu.ifi.dbs.elki.datasource.filter.normalization.columnwise package:} \]
Normalizations operating on columns / variates; where each column is treated independently.

Attribute Wise Beta Normalization
\[ \text{de.lmu.ifi.dbs.elki.datasource.filter.normalization.columnwise.AttributeWiseBetaNormalization} \] (since 0.7.0)
Project the data using a Beta distribution.
This is a crude heuristic, that may or may not work for your data set. There currently is no theoretical foundation of why it may be sensible or not to do this.

Attribute Wise CDF Normalization
\[ \text{de.lmu.ifi.dbs.elki.datasource.filter.normalization.columnwise.AttributeWiseCDFNormalization} \] (since 0.6.0)
Class to perform and undo a normalization on real vectors by estimating the distribution of values along each dimension independently, then rescaling objects to the cumulative density function (CDF) value at the original coordinate.
This process is for example also mentioned in section 3.4 of Effects of Feature Normalization on Image Retrieval S. Aksoy, R. M. Haralick but they do not detail how to obtain an appropriate function 'F'.

Attribute Wise MAD Normalization
\[ \text{de.lmu.ifi.dbs.elki.datasource.filter.normalization.columnwise.AttributeWiseMADNormalization} \] (since 0.6.0)
Median Absolute Deviation is used for scaling the data set as follows:
First, the median, and median absolute deviation are computed in each axis. Then, each value is projected to \((x - \text{median}(X)) / \text{MAD}(X)\).
This is similar to z-standardization of data sets, except that it is more robust towards outliers, and only slightly more expensive to compute.
**Attribute Wise Mean Normalization** (since 0.4.0)
de.lmu.ifi.dbs.elki.datasource.filter.normalization.columnwise.AttributeWiseMean

Normalization designed for data with a meaningful zero:
The 0 is retained, and the data is linearly scaled to have a mean of 1, by projection with $f(x) = x / \text{mean}(X)$. Each attribute is processed separately.

**Attribute Wise Min Max Normalization** (since 0.4.0)
de.lmu.ifi.dbs.elki.datasource.filter.normalization.columnwise.AttributeWiseMinMax

Class to perform and undo a normalization on real vectors with respect to a given minimum and maximum in each dimension. This class performs a linear scaling on the data.

**Attribute Wise Variance Normalization** (since 0.4.0)
de.lmu.ifi.dbs.elki.datasource.filter.normalization.columnwise.AttributeWiseVariance

Class to perform and undo a normalization on real vectors with respect to given mean and standard deviation in each dimension. We use the biased variance (MeanVariance.getNaiveStddev()), because this produces that with exactly standard deviation 1. While often the unbiased estimate (MeanVariance.getSampleStddev()) is more appropriate, it will not ensure this interesting property. For large data, the difference will be small anyway.

**Integer Rank Tie Normalization** (since 0.5.0)
de.lmu.ifi.dbs.elki.datasource.filter.normalization.columnwise.IntegerRankTie

Normalize vectors according to their rank in the attributes.
Note: ranks are multiplied by 2, to be able to give ties an integer rank. (e.g. when the first two records are tied, they both have rank "1" then, followed by the next on "4")

**Inverse Document Frequency Normalization** (since 0.4.0)
de.lmu.ifi.dbs.elki.datasource.filter.normalization.columnwise.InverseDocumentFrequency

Normalization for text frequency (TF) vectors, using the inverse document frequency (IDF). See also: TF-IDF for text analysis.

**Normalization Instancewise**

Instancewise normalization, where each instance is normalized independently.

**Hellinger Histogram Normalization** (since 0.7.0)
de.lmu.ifi.dbs.elki.datasource.filter.normalization.instancewise.HellingerHistogram

Normalize histograms by scaling them to unit absolute sum, then taking the square root of the absolute value in each attribute, times the normalization constant $1/\sqrt{2}$.

$$H(x_i) = \sqrt{\frac{|x_i|/\Sigma}{\sqrt{2}}}$$

with $\Sigma = \sum |x_i|

Using Euclidean distance (linear kernel) and this transformation is the same as using Hellinger distance: HellingerDistanceFunction

**Instance Log Rank Normalization** (since 0.7.0)
de.lmu.ifi.dbs.elki.datasource.filter.normalization.instancewise.InstanceLogRank

Normalize vectors such that the smallest value of each instance is 0, the largest is 1, but using $\log_2(1 + x)$.
Instance Mean Variance Normalization

Instance Min Max Normalization

Instance Rank Normalization

Length Normalization

Log1 Plus Normalization

By Label Filter

Random Sampling Stream Filter

Shuffle Objects Filter

Sort By Label Filter

Selection

Transform
Classic Multidimensional Scaling Transform
(de.lmu.ifi.dbs.elki.datasource.filter.transform.ClassicMultidimensionalScalingTransform)
Rescale the data set using multidimensional scaling, MDS.
Note: the current implementation is rather expensive, both memory- and runtime wise. Don't use for large data sets! Instead, have a look at FastMultidimensionalScalingTransform which uses power iterations instead.

Fast Multidimensional Scaling Transform
(de.lmu.ifi.dbs.elki.datasource.filter.transform.FastMultidimensionalScalingTransform)
Rescale the data set using multidimensional scaling, MDS.
This implementation uses power iterations, which is faster when the number of data points is much larger than the desired number of dimensions.
This implementation is $O(n^{3/2})$, and uses $O(n^{3/2})$ memory.

Global Principal Component Analysis Transform
(de.lmu.ifi.dbs.elki.datasource.filter.transform.GlobalPrincipalComponentAnalysisTransform)
Apply Principal Component Analysis (PCA) to the data set.
This is also popular form of "Whitening transformation", and will project the data to have a unit covariance matrix.
If you want to also reduce dimensionality, set the -pca.filter parameter! Note that this implementation currently will always perform a full matrix inversion. For very high dimensional data, this can take an excessive amount of time $O(d^3)$ and memory $O(d^3)$. Please contribute a better implementation to ELKI that only computes the required dimensions, yet allows for the same filtering flexibility.

Histogram Jitter Filter
(de.lmu.ifi.dbs.elki.datasource.filter.transform.HistogramJitterFilter)
Add Jitter, preserving the histogram properties (same sum, nonnegative).
For each vector, the total sum of all dimensions is computed.
Then a random vector of the average length $jitter \times scale$ is added and the result normalized to the original vectors sum. The individual dimensions are drawn from an exponential distribution with scale $jitter / \text{dimensionality}$, so it is expected that the error in most dimensions will be low, and higher in few.
This is designed to degrade the quality of a histogram, while preserving the total sum (e.g. to keep the normalization). The factor "jitter" can be used to control the degradation amount.

LatLngToECEF Filter
(de.lmu.ifi.dbs.elki.datasource.filter.transform.LatLngToECEFFilter)
Project a 2D data set (latitude, longitude) to a 3D coordinate system (X, Y, Z), such that Euclidean distance is line-of-sight.

Linear Discriminant Analysis Filter
(de.lmu.ifi.dbs.elki.datasource.filter.transform.LinearDiscriminantAnalysisFilter)
Linear Discriminant Analysis (LDA) / Fisher's linear discriminant.

LngLatToECEF Filter
(de.lmu.ifi.dbs.elki.datasource.filter.transform.LngLatToECEFFilter)
Project a 2D data set (longitude, latitude) to a 3D coordinate system (X, Y, Z), such that Euclidean distance is line-of-sight.

Number Vector Feature Selection Filter
(de.lmu.ifi.dbs.elki.datasource.filter.transform.NumberVectorFeatureSelectionFilter)
Parser to project the ParsingResult obtained by a suitable base parser onto a selected subset of attributes.
Number Vector Random Feature Selection Filter (since 0.4.0)
de.lmu.ifi.dbs.elki.datasource.filter.transform.NumberVectorRandomFeatureSelectionFilter
Parser to project the ParsingResult obtained by a suitable base parser onto a randomly selected subset of attributes.

Data Perturbation for Outlier Detection Ensembles [ZCS14] (since 0.7.0)
de.lmu.ifi.dbs.elki.datasource.filter.transform.PerturbationFilter
A filter to perturb the values by adding micro-noise. The added noise is generated, attribute-wise, by a Gaussian with mean=0 and a specified standard deviation or by a uniform distribution with a specified range. The standard deviation or the range can be scaled, attribute-wise, to a given percentage of the original standard deviation in the data distribution (assuming a Gaussian distribution there), or to a percentage of the extension in each attribute (maximumValue - minimumValue).
This filter has a potentially wide use but has been implemented for the following publication:

Projection Filter (since 0.6.0)
de.lmu.ifi.dbs.elki.datasource.filter.transform.ProjectionFilter
Apply a projection to the data.

E.1.5 Typeconversions
de.lmu.ifi.dbs.elki.datasource.filter.typeconversions package:
Filters to perform data type conversions.

Class Label Filter (since 0.4.0)
de.lmu.ifi.dbs.elki.datasource.filter.typeconversions.ClassLabelFilter
Class that turns a label column into a class label column.

Class Label From Pattern Filter (since 0.6.0)
de.lmu.ifi.dbs.elki.datasource.filter.typeconversions.ClassLabelFromPatternFilter
Streaming filter to derive an outlier class label.

External ID Filter (since 0.4.0)
de.lmu.ifi.dbs.elki.datasource.filter.typeconversions.ExternalIDFilter
Class that turns a label column into an external ID column.

Multivariate Time Series Filter (since 0.7.0)
de.lmu.ifi.dbs.elki.datasource.filter.typeconversions.MultivariateTimeSeriesFilter
Class to "fold" a flat number vector into a multivariate time series.

Sparse Vector Field Filter (since 0.5.0)
de.lmu.ifi.dbs.elki.datasource.filter.typeconversions.SparsesVectorFieldFilter
Class that turns sparse float vectors into a proper vector field, by setting the maximum dimensionality for each vector.

Split Number Vector Filter (since 0.4.0)
de.lmu.ifi.dbs.elki.datasource.filter.typeconversions.SplitNumberVectorFilter
Split an existing column into two types.

Uncertain Split Filter (since 0.7.0)
de.lmu.ifi.dbs.elki.datasource.filter.typeconversions.UncertainSplitFilter
Filter to transform a single vector into a set of samples to interpret as uncertain observation.
**Uncertainify Filter** (since 0.7.0)
de.lmu.ifi.dbs.elki.datasource.filter.typeconversions.UncertainifyFilter
Filter class to transform a database containing vector fields into a database containing UncertainObject fields by invoking a Uncertainifier on each vector.
The purpose for that is to use those transformed databases in experiments regarding uncertain data in some way.

**Weighted Uncertain Split Filter** (since 0.7.0)
de.lmu.ifi.dbs.elki.datasource.filter.typeconversions.WeightedUncertainSplitFilter
Filter to transform a single vector into a set of samples and weights to interpret as uncertain observation.

## E.2 Parser

de.lmu.ifi.dbs.elki.datasource.parser package:
Parsers for different file formats and data types.
The general use-case for any parser is to create objects out of an InputStream (e.g. by reading a data file). The objects are packed in a MultipleObjectsBundle which, in turn, is used by a DatabaseConnection-Object to fill a Database containing the corresponding objects.

By default (i.e., if the user does not specify any specific requests), any KDDTask will use the StaticArrayDatabase which, in turn, will use a FileBasedDatabaseConnection and a NumberVectorLabelParser to parse a specified data file creating a StaticArrayDatabase containing DoubleVector-Objects.

Thus, the standard procedure to use a data set of a real-valued vector space is to prepare the data set in a file of the following format (as suitable to NumberVectorLabelParser):

- One point per line, attributes separated by whitespace.
- Several labels may be given per point. A label must not be parseable as double.
- Lines starting with "#" will be ignored.
- An index can be specified to identify an entry to be treated as class label. This index counts all entries (numeric and labels as well) starting with 0.
- Files can be gzip compressed.

This file format is e.g. also suitable to gnuplot.

As an example file following these requirements consider e.g.: exampledata.txt

**ARFF File Format Parser** (since 0.4.0)
de.lmu.ifi.dbs.elki.datasource.parser.ArffParser
Parser to load WEKA .arff files into ELKI.
This parser is quite hackish, and contains lots of not yet configurable magic.

**Bit Vector Label Parser** (since 0.1)
de.lmu.ifi.dbs.elki.datasource.parser.BitVectorLabelParser
Parser for parsing one BitVector per line, bits separated by whitespace.
Several labels may be given per BitVector. A label must not be parseable as Bit. Lines starting with "#" will be ignored.

**CSV Reader Format** (since 0.1)
de.lmu.ifi.dbs.elki.datasource.parser.CSVReaderFormat
Basic format factory for parsing CSV-like formats.
To read CSV files into ELKI, see NumberVectorLabelParser.
This class encapsulates csv format settings, that need to be parsed in multiple places from ELKI, not only on input vector files.
Categorial Data As Number Vector Parser

A very simple parser for categorial data, which will then be encoded as numbers. This is closely modeled after the number vector parser.

Clustering Vector Parser

Parser for simple clustering results in vector form, as written by ClusteringVectorDumper. This allows reading the output of multiple clustering runs, and analyze the results using ELKI algorithm. The input format is very simple, each line containing a sequence of cluster assignments in integer form, and an optional label:

0 0 1 1 0 First  
0 0 0 1 2 Second

represents two clusterings for 5 objects. The first clustering has two clusters, the second contains three clusters.

libSVM Format Parser

Parser to read libSVM format files. The format of libSVM is roughly specified in the README given:

<i>label</i> <i>index1</i>:<i>value1</i> <i>index2</i>:<i>value2</i> ...

i.e. a mandatory integer class label in the beginning followed by a classic sparse vector representation of the data. indexes are integers, starting at 1 (Note that ELKI uses 0-based indexing, so we will map these to index-1) to not always have a constant-0 dimension 0.

The libSVM FAQ states that you can also put comments into the file, separated by a hash: #, but they must not contain colons and are not officially supported. ELKI will simply stop parsing a line when encountering a #.

Number Vector Label Parser

Parser for a simple CSV type of format, with columns separated by the given pattern (default: whitespace). Several labels may be given per point. A label must not be parseable as double. Lines starting with "#" will be ignored.

An index can be specified to identify an entry to be treated as class label. This index counts all entries (numeric and labels as well) starting with 0.

Simple Polygon Parser

Parser to load polygon data (2D and 3D only) from a simple format. One record per line, points separated by whitespace, numbers separated by colons. Multiple polygons components can be separated using -.

Unparseable parts will be treated as labels.

Simple Transaction Parser

Simple parser for transactional data, such as market baskets. To keep the input format simple and readable, all tokens are assumed to be of text and separated by whitespace, and each transaction is on a separate line.

An example file containing two transactions looks like this

bread butter milk  
paste tomato basil
Sparse Vector Label Parser

Parser for parsing one point per line, attributes separated by whitespace.
Several labels may be given per point. A label must not be parseable as double. Lines starting with "#" will be ignored.

A line is expected in the following format: The first entry of each line is the number of attributes with coordinate value not zero. Subsequent entries are of the form index value each, where index is the number of the corresponding dimension, and value is the value of the corresponding attribute. A complete line then could look like this:
3 7 12.34 8 56.78 11 1.234 objectlabel
where 3 indicates there are three attributes set, 7,8,11 are the attributes indexes and there is a non-numerical object label.
An index can be specified to identify an entry to be treated as class label. This index counts all entries (numeric and labels as well) starting with 0.

String Parser

Parser that loads a text file for use with string similarity measures.
The parser produces two relations: the first of type String, the second of type label list, which contains the same data for convenience.

Term Frequency Parser

A parser to load term frequency data, which essentially are sparse vectors with text keys.
Parse a file containing term frequencies. The expected format is:
rowlabel1 term1 <freq> term2 <freq> ...
rowlabel2 term1 <freq> term3 <freq> ...
Terms must not contain the separator character!
If your data does not contain frequencies, you can maybe use SimpleTransactionParser instead.

F Distance

de.lmu.ifi.dbs.elki.distance package:

F.1 Distancefunction

de.lmu.ifi.dbs.elki.distance.distancefunction package:
Distance functions for use within ELKI.

Distance functions

There are three basic types of distance functions:
• Primitive Distance Functions that can be computed for any two objects.
• DBID Distance Functions, that are only defined for object IDs, e.g. an external distance matrix
• Index-Based Distance Functions, that require an indexing/preprocessing step, and are then valid for existing database objects.
These types differ significantly in both implementation and use.

Using distance functions

As a 'consumer' of distances, you usually do not care about the type of distance function you want to use. To facilitate this, a distance function can be bound to a database by calling the 'instantiate' method to obtain a DistanceQuery object. A distance query is a best-effort adapter for the given distance function.
Usually, you pass it two DBIDs and get the distance value back. When required, the adapter will get the appropriate records from the database needed to compute the distance.

Note: instantiating a preprocessor based distance will invoke the preprocessing step. It is recommended to do this as soon as possible, and only instantiate the query once, then pass the query object through the various methods.

**Code example**

```java
DistanceQuery<V> distanceQuery = database.getDistanceQuery(EuclideanDistanceFunction.STATIC);
```

### Arc Cosine Distance Function  (since 0.2)

Arcus cosine distance function for feature vectors.

The arc cosine distance is computed as the arcus from the cosine similarity value, i.e., \( \arccos(<v_1,v_2>) \). Cosine similarity is defined as:

\[
\frac{\mathbf{x} \cdot \mathbf{y}}{||a|| \cdot ||b||}
\]

Arcus cosine distance then is

\[
\arccos \frac{\mathbf{x} \cdot \mathbf{y}}{||a|| \cdot ||b||} \in [0; \pi]
\]

`CosineDistanceFunction` is a bit less expensive, and will yield the same ranking of neighbors.

### Arc Cosine Unitlength Distance Function  (since 0.7.5)

Arcus cosine distance function for feature vectors.

The arc cosine distance is computed as the arcus from the cosine similarity value, i.e., \( \arccos(<v_1,v_2>) \). Cosine similarity is defined as:

\[
\frac{\mathbf{x} \cdot \mathbf{y}}{||a|| \cdot ||b||} = ||a|| = ||b|| = 1 \\| \mathbf{x} \\|.\| \mathbf{y} \|
\]

Arcus cosine distance then is

\[
\arccos \frac{\mathbf{x} \cdot \mathbf{y}}{||a|| \cdot ||b||} = ||a|| = ||b|| = 1 \arccos \frac{\mathbf{x} \cdot \mathbf{y}}{1} \in [0; \pi]
\]

This implementation assumes that \( ||a|| = ||b|| = 1 \). If this does not hold for your data, use `ArcCosineDistanceFunction` instead!

`CosineUnitlengthDistanceFunction` is a bit less expensive, and will yield the same ranking of neighbors.

### Bray Curtis Distance Function  \([\text{So48, BC57, Dic45}]\)  (since 0.6.0)

Bray-Curtis distance function / Sørensen–Dice coefficient for continuous vector spaces (not only binary data).

### Canberra Distance Function  \([LW66]\)  (since 0.5.0)

Canberra distance function, a variation of Manhattan distance.

Canberra distance is defined as:

\[
\text{Canberra}(\mathbf{x}, \mathbf{y}) := \sum_i \frac{|x_i-y_i|}{|x_i|+|y_i|}
\]

### Clark Distance Function  \([\text{DL09}]\)  (since 0.6.0)

Clark distance function for vector spaces.

Clark distance is defined as:

\[
\text{Clark}(\mathbf{x}, \mathbf{y}) := \sqrt{\frac{1}{2} \sum_i \left( \frac{|x_i-y_i|}{|x_i|+|y_i|} \right)^2}
\]
Cosine Distance Function

department of informatics, university of munich.\texttt{CosineDistanceFunction} (since 0.1)

Cosine distance function for feature vectors.

The cosine distance is computed from the cosine similarity by $1 - \text{cosine similarity}$.

Cosine similarity is defined as

$$\frac{\vec{x} \cdot \vec{y}}{||a|| \cdot ||b||}$$

Cosine distance then is defined as

$$1 - \frac{\vec{x} \cdot \vec{y}}{||a|| \cdot ||b||} \in [0; 2]$$

\texttt{ArcCosineDistanceFunction} may sometimes be more appropriate, but also more computationally expensive.

Cosine Unitlength Distance Function

department of informatics, university of munich.\texttt{CosineUnitlengthDistanceFunction} (since 0.7.5)

Cosine distance function for unit length feature vectors.

The cosine distance is computed from the cosine similarity by $1 - \text{cosine similarity}$.

Cosine similarity is defined as

$$\frac{\vec{x} \cdot \vec{y}}{||a|| \cdot ||b||} = \frac{1}{||a||} = \frac{1}{||b||}$$

Cosine distance then is defined as

$$1 - \frac{\vec{x} \cdot \vec{y}}{||a|| \cdot ||b||} = \frac{1}{||a||} = \frac{1}{||b||} \in [0; 2]$$

This implementation assumes that $||a|| = ||b|| = 1$. If this does not hold for your data, use \texttt{CosineDistanceFunction} instead!

\texttt{ArcCosineUnitlengthDistanceFunction} may sometimes be more appropriate, but also more computationally expensive.

Mahalanobis Distance Function

department of informatics, university of munich.\texttt{MahalanobisDistanceFunction} (since 0.7.5)

Mahalanobis quadratic form distance for feature vectors.

For a weight matrix $M$, this distance is defined as

$$\text{Mahalanobis}_M(x, y) := \sqrt{(x - y)^T \cdot M \cdot (x - y)}$$

Random Stable Distance Function

department of informatics, university of munich.\texttt{RandomStableDistanceFunction} (since 0.4.0)

This is a dummy distance providing random values (obviously not metrical), useful mostly for unit tests and baseline evaluations: obviously this distance provides no benefit whatsoever.

This distance is based on the combined hash codes of the two objects queried, if they are different. Extra caution is done to ensure symmetry and objects with the same ID will have a distance of 0. Obviously this distance is not metrical.

Shared Nearest Neighbor Jaccard Distance Function

department of informatics, university of munich.\texttt{SharedNearestNeighborJaccardDistanceFunction} (since 0.4.0)

\texttt{SharedNearestNeighborJaccardDistanceFunction} computes the Jaccard coefficient, which is a proper distance metric.

Weighted Canberra Distance Function

department of informatics, university of munich.\texttt{WeightedCanberraDistanceFunction} (since 0.5.0)

Weighted Canberra distance function, a variation of Manhattan distance.

F.1.1 Adapter

department of informatics, university of munich.\texttt{adapter} package:

Distance functions deriving distances from e.g. similarity measures
**Arccos Similarity Adapter**

(de.lmu.ifi.dbs.elki.distance.distancefunction.adapter.ArccosSimilarityAdapter)

Adapter from a normalized similarity function to a distance function using \( \arccos(sim) \).

**Linear Adapter Linear**

(de.lmu.ifi.dbs.elki.distance.distancefunction.adapter.LinearAdapterLinear)

Adapter from a normalized similarity function to a distance function using \( 1 - sim \).

**Ln Similarity Adapter**

(de.lmu.ifi.dbs.elki.distance.distancefunction.adapter.LnSimilarityAdapter)

Adapter from a normalized similarity function to a distance function using \( -\log(sim) \).

**F.1.2 Colorhistogram**

(de.lmu.ifi.dbs.elki.distance.distancefunction.colorhistogram package:)

Distance functions using correlations.

**HSB Histogram Quadratic Distance Function**

[SC96] (since 0.3)

(de.lmu.ifi.dbs.elki.distance.distancefunction.colorhistogram.HSBHistogramQuadraticDistanceFunction)

Distance function for HSB color histograms based on a quadratic form and color similarity. The matrix is filled according to:

VisualSEEK: a fully automated content-based image query system
J. R. Smith, S. F. Chang
Proc. 4th ACM Int. Conf. on Multimedia 1997

**Histogram Intersection Distance Function**

[SB91] (since 0.3)

(de.lmu.ifi.dbs.elki.distance.distancefunction.colorhistogram.HistogramIntersectionDistanceFunction)

Intersection distance for color histograms.
Distance function for color histograms that emphasizes 'strong' bins.

**RGB Histogram Quadratic Distance Function**

[HSE+95] (since 0.3)

(de.lmu.ifi.dbs.elki.distance.distancefunction.colorhistogram.RGBHistogramQuadraticDistanceFunction)

Distance function for RGB color histograms based on a quadratic form and color similarity.

**F.1.3 Correlation**

(de.lmu.ifi.dbs.elki.distance.distancefunction.correlation package:)

Distance functions using correlations.

**Absolute Pearson Correlation Distance Function**

(since 0.7.0)

(de.lmu.ifi.dbs.elki.distance.distancefunction.correlation.AbsolutePearsonCorrelationDistanceFunction)

Absolute Pearson correlation distance function for feature vectors.
The absolute Pearson correlation distance is computed from the Pearson correlation coefficient \( r \) as: \( 1 - \text{abs}(r) \).
The distance between two vectors will be low (near 0), if their attribute values are dimension-wise strictly positively or negatively correlated, it will be high (near 1), if their attribute values are dimension-wise uncorrelated.
Absolute Uncentered Correlation Distance Function (since 0.7.0)

de.lmu.ifi.dbs.elki.distance.distancefunction.correlation.AbsoluteUncenteredCorrelationDistanceFunction

Absolute uncentered correlation distance function for feature vectors.
This is highly similar to AbsolutePearsonCorrelationDistanceFunction, but uses a fixed mean of 0 instead of the sample mean.

Pearson Correlation Distance Function (since 0.3)

de.lmu.ifi.dbs.elki.distance.distancefunction.correlation.PearsonCorrelationDistanceFunction

Pearson correlation distance function for feature vectors.
The Pearson correlation distance is computed from the Pearson correlation coefficient $r$ as: $1-r$. Hence, possible values of this distance are between 0 and 2.
The distance between two vectors will be low (near 0), if their attribute values are dimension-wise strictly positively correlated, it will be high (near 2), if their attribute values are dimension-wise strictly negatively correlated. For Features with uncorrelated attributes, the distance value will be intermediate (around 1).

Squared Pearson Correlation Distance Function (since 0.3)

de.lmu.ifi.dbs.elki.distance.distancefunction.correlation.SquaredPearsonCorrelationDistanceFunction

Squared Pearson correlation distance function for feature vectors.
The squared Pearson correlation distance is computed from the Pearson correlation coefficient $r$ as: $1-r^2$. Hence, possible values of this distance are between 0 and 1.
The distance between two vectors will be low (near 0), if their attribute values are dimension-wise strictly positively or negatively correlated. For features with uncorrelated attributes, the distance value will be high (near 1).

Squared Uncentered Correlation Distance Function (since 0.7.0)

de.lmu.ifi.dbs.elki.distance.distancefunction.correlation.SquaredUncenteredCorrelationDistanceFunction

Squared uncentered correlation distance function for feature vectors.
This is highly similar to SquaredPearsonCorrelationDistanceFunction, but uses a fixed mean of 0 instead of the sample mean.

Uncentered Correlation Distance Function (since 0.7.0)

de.lmu.ifi.dbs.elki.distance.distancefunction.correlation.UncenteredCorrelationDistanceFunction

Uncentered correlation distance.
This is highly similar to PearsonCorrelationDistanceFunction, but uses a fixed mean of 0 instead of the sample mean.

Weighted Pearson Correlation Distance Function (since 0.4.0)

de.lmu.ifi.dbs.elki.distance.distancefunction.correlation.WeightedPearsonCorrelationDistanceFunction

Pearson correlation distance function for feature vectors.
The Pearson correlation distance is computed from the Pearson correlation coefficient $r$ as: $1-r$. Hence, possible values of this distance are between 0 and 2.
The distance between two vectors will be low (near 0), if their attribute values are dimension-wise strictly positively correlated, it will be high (near 2), if their attribute values are dimension-wise strictly negatively correlated. For Features with uncorrelated attributes, the distance value will be intermediate (around 1).
This variation is for weighted dimensions.
Weighted Squared Pearson Correlation Distance Function (since 0.4.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.correlation.WeightedSquaredPearsonCorrelationDistanceFunction

Weighted squared Pearson correlation distance function for feature vectors.
The squared Pearson correlation distance is computed from the Pearson correlation coefficient $r$ as $1 - r^2$.
Hence, possible values of this distance are between 0 and 1.
The distance between two vectors will be low (near 0), if their attribute values are dimension-wise strictly positively or negatively correlated. For features with uncorrelated attributes, the distance value will be high (near 1).
This variation is for weighted dimensions.

F.1.4 External
de.lmu.ifi.dbs.elki.distance.distancefunction.external package:
Distance functions using external data sources.

Ascii Distance Parser (since 0.1)
de.lmu.ifi.dbs.elki.distance.distancefunction.externalAsciiDistanceParser
Parser for parsing one distance value per line.
A line must have the following format: id1 id2 distanceValue, where id1 and id2 are integers starting at 0 representing the two ids belonging to the distance value. Lines starting with "#" will be ignored.

Disk Cache Based Double Distance Function (since 0.2)
de.lmu.ifi.dbs.elki.distance.distancefunction.externalDiskCacheBasedDoubleDistanceFunction
Distance function that is based on double distances given by a distance matrix of an external binary matrix file.

Disk Cache Based Float Distance Function (since 0.2)
de.lmu.ifi.dbs.elki.distance.distancefunction.externalDiskCacheBasedFloatDistanceFunction
Distance function that is based on float distances given by a distance matrix of an external binary matrix file.

File Based Sparse Double Distance Function (since 0.1)
de.lmu.ifi.dbs.elki.distance.distancefunction.externalFileBasedSparseDoubleDistanceFunction
Distance function that is based on double distances given by a distance matrix of an external ASCII file.
Note: parsing an ASCII file is rather expensive.
See AsciiDistanceParser for the default input format.

File Based Sparse Float Distance Function (since 0.1)
de.lmu.ifi.dbs.elki.distance.distancefunction.externalFileBasedSparseFloatDistanceFunction
Distance function that is based on float distances given by a distance matrix of an external ASCII file.
Note: parsing an ASCII file is rather expensive.
See AsciiDistanceParser for the default input format.

F.1.5 Geo
de.lmu.ifi.dbs.elki.distance.distancefunction.geo package:
Geographic (earth) distance functions.
Dimension Selecting Lat Lng Distance Function \[\text{SZK13}\] (since 0.4.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.geo.DimensionSelectingLatLngDistanceFunction
Distance function for 2D vectors in Latitude, Longitude form.
The input data must be in degrees (not radians), and the output distance will be in meters (see EarthModel.distanceDeg(double, double, double, double)).
This implementation allows index accelerated queries using R*-trees (by providing a point-to-rectangle minimum distance).

LatLng Distance Function \[\text{SZK13}\] (since 0.4.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.geo.LatLngDistanceFunction
Distance function for 2D vectors in Latitude, Longitude form.
The input data must be in degrees (not radians), and the output distance will be in meters (see EarthModel.distanceDeg(double, double, double, double)).
This implementation allows index accelerated queries using R*-trees (by providing a point-to-rectangle minimum distance).

LngLat Distance Function \[\text{SZK13}\] (since 0.4.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.geo.LngLatDistanceFunction
Distance function for 2D vectors in Longitude, Latitude form.
The input data must be in degrees (not radians), and the output distance will be in meters (see EarthModel.distanceDeg(double, double, double, double)).
This implementation allows index accelerated queries using R*-trees (by providing a point-to-rectangle minimum distance).

F.1.6 Histogram
de.lmu.ifi.dbs.elki.distance.distancefunction.histogram package:
Distance functions for one-dimensional histograms.

Histogram Match Distance Function \[\text{Vas69}\] (since 0.6.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.histogram.HistogramMatchDistanceFunction
Distance function based on histogram matching, i.e. Manhattan distance on the cumulative density function.
This distance function assumes there exist a natural order in the vectors, i.e. they should be some 1-dimensional histogram.
This is also known as Earth Movers Distance (EMD), 1st Mallows distance or 1st Wasserstein metric (also Vasershtein metric), for the special case of a one-dimensional histogram, where the cost is linear in the number of bins to transport.

Kolmogorov Smirnov Distance Function
\[(\text{since 0.6.0})\]
de.lmu.ifi.dbs.elki.distance.distancefunction.histogram.KolmogorovSmirnovDistanceFunction
Distance function based on the Kolmogorov-Smirnov goodness of fit test.
This distance function assumes there exist a natural order in the vectors, i.e. they should be some 1-dimensional histogram.

F.1.7 Minkowski
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski package:
Minkowski space $L_p$ norms such as the popular Euclidean and Manhattan distances.
**Euclidean Distance Function** (since 0.1)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.EuclideanDistanceFunction

Euclidean distance for NumberVectors.

Euclidean distance is defined as:

\[
euclidean(\vec{x}, \vec{y}) := \sqrt{\sum_i (x_i - y_i)^2}
\]

**LP Norm Distance Function** (since 0.1)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.LPNormDistanceFunction

L_p-Norm (Minkowski norms) are a family of distances for NumberVectors.

The L_p distance is defined as:

\[
L_p(\vec{x}, \vec{y}) := \left(\sum_i (x_i - y_i)\right)^{1/p}
\]

For p >= 1 this is a metric. For p=1, this yields the well known ManhattanDistanceFunction, for p = 2 the standard EuclideanDistanceFunction.

**Manhattan Distance Function** (since 0.1)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.ManhattanDistanceFunction

Manhattan distance for NumberVectors.

Manhattan distance is defined as:

\[
manhattan(\vec{x}, \vec{y}) := \sum_i |x_i - y_i|
\]

**Maximum Distance Function** (since 0.3)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.MaximumDistanceFunction

Maximum distance for NumberVectors.

The maximum distance is defined as:

\[
\text{Maximum}(\vec{x}, \vec{y}) := \max_i |x_i - y_i|
\]

and can be seen as limiting case of the LPNormDistanceFunction for \( p \to \infty \).

**Minimum Distance Function** (since 0.3)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.MinimumDistanceFunction

Minimum distance for NumberVectors.

Minimum distance is defined as:

\[
\text{Minimum}_p(\vec{x}, \vec{y}) := \min_i |x_i - y_i|
\]

This is not a metric, but can sometimes be useful as a lower bound.

**Sparse Euclidean Distance Function** (since 0.5.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.SparseEuclideanDistanceFunction

Euclidean distance function, optimized for SparseNumberVectors.

Euclidean distance is defined as:

\[
euclidean(\vec{x}, \vec{y}) := \sqrt{\sum_i (x_i - y_i)^2}
\]

For sparse vectors, we can skip those \( i \) where both vectors are 0.

**Sparse LP Norm Distance Function** (since 0.5.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.SparseLPNormDistanceFunction

L_p-Norm, optimized for SparseNumberVectors.

The L_p distance is defined as:

\[
L_p(\vec{x}, \vec{y}) := \left(\sum_i (x_i - y_i)\right)^{1/p}
\]
Sparse Manhattan Distance Function (since 0.5.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.SparseManhattanDistanceFunction
Manhattan distance, optimized for SparseNumberVectors.
Manhattan distance is defined as:
\[
\text{Manhattan}(\vec{x}, \vec{y}) := \sum_i |x_i - y_i|
\]

Sparse Maximum Distance Function (since 0.5.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.SparseMaximumDistanceFunction
Maximum distance, optimized for SparseNumberVectors.
The maximum distance is defined as:
\[
\text{Maximum}(\vec{x}, \vec{y}) := \max_i |x_i - y_i|
\]
and can be seen as limiting case of the LPNormDistanceFunction for \( p \to \infty \).

Squared Euclidean Distance Function (since 0.1)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.SquaredEuclideanDistanceFunction
Squared Euclidean distance, optimized for SparseNumberVectors. This results in the same rankings as regular Euclidean distance, but saves computing the square root.
Squared Euclidean is defined as:
\[
\text{Euclidean}^2(\vec{x}, \vec{y}) := \sum_i (x_i - y_i)^2
\]

Weighted Euclidean Distance Function (since 0.4.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.WeightedEuclideanDistanceFunction
Weighted Euclidean distance for NumberVectors.
Weighted Euclidean distance is defined as:
\[
\text{Euclidean}_w(\vec{x}, \vec{y}) := \sqrt{\sum_i w_i (x_i - y_i)^2}
\]

Weighted LP Norm Distance Function (since 0.4.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.WeightedLPNormDistanceFunction
Weighted version of the Minkowski \( L_p \) norm distance for NumberVector.
Weighted \( L_p \) Norms are defined as:
\[
L_{p,w}(\vec{x}, \vec{y}) := \left( \sum_i w_i |x_i - y_i|^p \right)^{1/p}
\]

Weighted Manhattan Distance Function (since 0.4.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.WeightedManhattanDistanceFunction
Weighted version of the Manhattan (\( L_1 \)) metric.
Weighted Manhattan distance is defined as:
\[
\text{Manhattan}_w(\vec{x}, \vec{y}) := \sum_i w_i |x_i - y_i|
\]

Weighted Maximum Distance Function (since 0.6.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.minkowski.WeightedMaximumDistanceFunction
Weighted version of the maximum distance function for NumberVectors.
Weighted maximum distance is defined as:
\[
\text{Maximum}_w(\vec{x}, \vec{y}) := \max_i w_i |x_i - y_i|
\]
Weighted Squared Euclidean Distance Function

Weighted squared Euclidean distance for `NumberVectors`. This results in the same rankings as weighted Euclidean distance, but saves computing the square root.

Weighted squared Euclidean is defined as:

\[
\text{Euclidean}^2_w(\vec{x}, \vec{y}) := \sum_i w_i (x_i - y_i)^2
\]

F.1.8 Probabilistic

Distance from probability theory, mostly divergences such as K-L-divergence, J-divergence, F-divergence, \(\chi^2\)-divergence, etc.

Chi Distance Function \([ES03, PRTB99]\) (since 0.7.5)

Chi distance function, symmetric version. This is the square root of the ChiSquaredDistanceFunction, and can serve as a fast approximation to SqrtJensenShannonDivergenceDistanceFunction.

This implementation assumes \(\sum_i x_i = \sum_i y_i\), and is defined as:

\[
\chi(\vec{x}, \vec{y}) := \sqrt{2 \sum_i \frac{(x_i - y_i)^2}{x_i + y_i}}
\]

Chi Squared Distance Function \([PRTB99]\) (since 0.6.0)

\(\chi^2\) distance function, symmetric version.

This implementation assumes \(\sum_i x_i = \sum_i y_i\), and is defined as:

\[
\chi^2(\vec{x}, \vec{y}) := 2 \sum_i \frac{(x_i - y_i)^2}{x_i + y_i}
\]

Fisher Rao Distance Function \([DD09, Rao45]\) (since 0.7.5)

Fisher-Rao riemannian metric for (discrete) probability distributions.

\[
\text{Fisher-Rao}(\vec{x}, \vec{y}) := 2 \arccos \sum_i \sqrt{x_i y_i}
\]

Hellinger Distance Function \([DD09, Hel09]\) (since 0.7.0)

Hellinger metric / affinity / kernel, Bhattacharyya coefficient, fidelity similarity, Matusita distance, Hellinger-Kakutani metric on a probability distribution.

We assume vectors represent normalized probability distributions. Then

\[
\text{Hellinger}(\vec{x}, \vec{y}) := \sqrt{\frac{1}{2} \sum_i (\sqrt{x_i} - \sqrt{y_i})^2}
\]

The corresponding kernel / similarity is

\[
K_{\text{Hellinger}}(\vec{x}, \vec{y}) := \sum_i \sqrt{x_i y_i}
\]

If we have normalized probability distributions, we have the nice property that \(K_{\text{Hellinger}}(\vec{x}, \vec{x}) = \sum_i x_i = 1\). and therefore \(K_{\text{Hellinger}}(\vec{x}, \vec{y}) \in [0; 1]\).

Furthermore, we have the following relationship between this variant of the distance and this kernel:

\[
\text{Hellinger}^2(\vec{x}, \vec{y}) = \frac{1}{2} \sum_i (\sqrt{x_i} - \sqrt{y_i})^2 = \frac{1}{2} \sum_i x_i + y_i - 2 \sqrt{x_i y_i}
\]

\[
\text{Hellinger}^2(\vec{x}, \vec{y}) = \frac{1}{2} K_{\text{Hellinger}}(\vec{x}, \vec{x}) + \frac{1}{2} K_{\text{Hellinger}}(\vec{y}, \vec{y}) - K_{\text{Hellinger}}(\vec{x}, \vec{y}) = 1 - K_{\text{Hellinger}}(\vec{x}, \vec{y})
\]

which implies \(\text{Hellinger}(\vec{x}, \vec{y}) \in [0; 1]\), and is very similar to the Euclidean distance and the linear kernel.
From this, it follows trivially that Hellinger distance corresponds to the kernel transformation $\phi : \vec{x} \mapsto (\sqrt{\frac{x_1}{2}}, \ldots, \sqrt{\frac{x_d}{2}})$.

Deza and Deza unfortunately also give a second definition, as:

$$\text{Hellinger-Deza}(\vec{x}, \vec{y}) := \sqrt{2 \sum_i (\sqrt{\frac{x_i}{2}} - \sqrt{\frac{y_i}{2}})^2}$$

which has a built-in normalization, and a different scaling that is no longer bound to $[0; 1]$. The 2 in this definition likely should be $\frac{1}{2}$.

This distance is well suited for histograms, but it is then more efficient to once normalize the histograms, apply the square roots, and then use Euclidean distance (i.e., use the "kernel trick" in reverse, materializing the transformation $\phi$ given above).

**Jeffrey Divergence Distance Function**

**Kullback Leibler Divergence Asymmetric Distance Function**

**Kullback Leibler Divergence Reverse Asymmetric Distance Function**

**Jensen Shannon Divergence Distance Function**
**Sqrt Jensen Shannon Divergence Distance Function** [ES03] (since 0.6.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.probabilistic.SqrtJensenShannonDivergenceDistanceFunction

The square root of Jensen-Shannon divergence is a metric.

\[ \sqrt{JS(x, y)} := \sqrt{\frac{1}{2} \sum_i x_i \log \frac{2x_i}{x_i+y_i} + y_i \log \frac{2y_i}{x_i+y_i}} = \sqrt{JS(x, y)} \]

A proof of triangle inequality (for "\(D_{PQ}\)") can be found in Endres and Schindelin.

**Triangular Discrimination Distance Function** [Top00] (since 0.7.5)
de.lmu.ifi.dbs.elki.distance.distancefunction.probabilistic.TriangularDiscriminationDistanceFunction

Triangular Discrimination has relatively tight upper and lower bounds to the Jensen-Shannon divergence, but is much less expensive.

\[ \text{Triangular-Discrimination}(x, y) := \sum_i |x_i - y_i|^2 \]

This distance function is meant for distribution vectors that sum to 1, and does not work on negative values.

See also TriangularDistanceFunction for a metric version.

**Triangular Distance Function** [CCVR16] (since 0.7.5)
de.lmu.ifi.dbs.elki.distance.distancefunction.probabilistic.TriangularDistanceFunction

Triangular Distance has relatively tight upper and lower bounds to the (square root of the) Jensen-Shannon divergence, but is much less expensive.

\[ \text{Triangular-Distance}(x, y) := \sqrt{\sum_i |x_i - y_i|^2} \]

This distance function is meant for distribution vectors that sum to 1, and does not work on negative values.

This differs from TriangularDistanceFunction simply by the square root, which makes it a proper metric and a good approximation for the much more expensive SqrtJensenShannonDivergenceDistanceFunction.

**F.1.9 Set**
de.lmu.ifi.dbs.elki.distance.distancefunction.set package:
Distance functions for binary and set type data.

**Hamming Distance Function** [Ham50] (since 0.7.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.set.HammingDistanceFunction

Computes the Hamming distance of arbitrary vectors - i.e. counting, on how many places they differ.

**Jaccard Similarity Distance Function** [Jac02] (since 0.6.0)
de.lmu.ifi.dbs.elki.distance.distancefunction.set.JaccardSimilarityDistanceFunction

A flexible extension of Jaccard similarity to non-binary vectors.

Jaccard coefficient is commonly defined as \(\frac{|A \cap B|}{|A \cup B|}\).

We can extend this definition to non-binary vectors as follows: \(\frac{|\{i|a_i=b_i\}|}{|\{i|a_i=0\} \cup |\{i|b_i=0\}|}\)

For binary vectors, this will obviously be the same quantity. However, this version is more useful for categorical data.

**F.1.10 Strings**
de.lmu.ifi.dbs.elki.distance.distancefunction.strings package:
Distance functions for strings.
Levenshtein Distance Function [Lev66] (since 0.6.0)
dep.lmu.ifi.dbs.elki.distance.distancefunction.strings.LevenshteinDistanceFunction
Classic Levenshtein distance on strings.

Normalized Levenshtein Distance Function [Lev66] (since 0.6.0)
dep.lmu.ifi.dbs.elki.distance.distancefunction.strings.NormalizedLevenshteinDistanceFunction
Levenshtein distance on strings, normalized by string length.
Note: this is no longer a metric, the triangle inequality is violated. Example: \(d("ab","bc")=1, d("ab","abc")+d("abc","bc")=0.4+0.4=0.8\)

F.1.11 Subspace
dep.lmu.ifi.dbs.elki.distance.distancefunction.subspace package:
Distance functions based on subspaces.

Onedimensional Distance Function (since 0.1)
dep.lmu.ifi.dbs.elki.distance.distancefunction.subspace.OnedimensionalDistanceFunction
Distance function that computes the distance between feature vectors as the absolute difference of their values in a specified dimension only.

Subspace Euclidean Distance Function (since 0.1)
dep.lmu.ifi.dbs.elki.distance.distancefunction.subspace.SubspaceEuclideanDistanceFunction
Euclidean distance function between NumberVectors only in specified dimensions.

Subspace LP Norm Distance Function (since 0.1)
dep.lmu.ifi.dbs.elki.distance.distancefunction.subspace.SubspaceLPNormDistanceFunction
L_p-Norm distance function between NumberVectors only in specified dimensions.

Subspace Manhattan Distance Function (since 0.1)
dep.lmu.ifi.dbs.elki.distance.distancefunction.subspace.SubspaceManhattanDistanceFunction
Manhattan distance function between NumberVectors only in specified dimensions.

Subspace Maximum Distance Function (since 0.1)
dep.lmu.ifi.dbs.elki.distance.distancefunction.subspace.SubspaceMaximumDistanceFunction
Maximum distance function between NumberVectors only in specified dimensions.

F.1.12 Timeseries
dep.lmu.ifi.dbs.elki.distance.distancefunction.timeseries package:
Distance functions designed for time series.
Note that some regular distance functions (e.g. Euclidean) are also used on time series.

Dynamic Time Warping Distance Function [BC94] (since 0.2)
dep.lmu.ifi.dbs.elki.distance.distancefunction.timeseries.DTWDistanceFunction
Dynamic Time Warping distance (DTW) for numerical vectors.

Derivative dynamic time warping [KP01] (since 0.7.0)
dep.lmu.ifi.dbs.elki.distance.distancefunction.timeseries.DerivativeDTWDistanceFunction
Derivative Dynamic Time Warping distance for numerical vectors.
Edit Distance on Real Sequence \[\text{COO05}\] \text{(since 0.2)}
de.lmu.ifi.dbs.elki.distance.distancefunction.timeseries.\text{EDRDistanceFunction}
Edit Distance on Real Sequence distance for numerical vectors.

Edit Distance with Real Penalty \[\text{CN04}\] \text{(since 0.2)}
de.lmu.ifi.dbs.elki.distance.distancefunction.timeseries.\text{ERPDistanceFunction}
Edit Distance With Real Penalty distance for numerical vectors.

Longest Common Subsequence distance function \[\text{VHGK03}\] \text{(since 0.2)}
de.lmu.ifi.dbs.elki.distance.distancefunction.timeseries.\text{LCSSDistanceFunction}
Longest Common Subsequence distance for numerical vectors.
Originally this was based on the Matlab Code by Michalis Vlachos, but we have since switched to a version that uses less memory.

F.2 Similarity function
de.lmu.ifi.dbs.elki.distance.\text{similarityfunction} \text{package:}
Similarity functions.

Fractional Shared Nearest Neighbor Similarity Function \text{(since 0.2)}
de.lmu.ifi.dbs.elki.distance.similarityfunction.\text{FractionalSharedNearestNeighborSimilarityFunction}
SharedNearestNeighborSimilarityFunction with a pattern defined to accept Strings that define a non-negative Integer.

Inverted Distance Similarity Function \text{(since 0.5.0)}
de.lmu.ifi.dbs.elki.distance.similarityfunction.\text{InvertedDistanceSimilarityFunction}
Adapter to use a primitive number-distance as similarity measure, by computing 1/distance.

Kulczynski 1 Similarity Function \[\text{DD09}\] \text{(since 0.6.0)}
de.lmu.ifi.dbs.elki.distance.similarityfunction.\text{Kulczynski1SimilarityFunction}
Kulczynski similarity 1.
\[s_{\text{Kulczynski-1}}(\vec{x}, \vec{y}) := \sum_i \min\{x_i, y_i\}\]
or in distance form:
\[d_{\text{Kulczynski-1}}(\vec{x}, \vec{y}) := \sum_i \min\{x_i, y_i\}\]

Kulczynski 2 Similarity Function \[\text{DD09}\] \text{(since 0.6.0)}
de.lmu.ifi.dbs.elki.distance.similarityfunction.\text{Kulczynski2SimilarityFunction}
Kulczynski similarity 2.
\[s_{\text{Kulczynski-2}}(\vec{x}, \vec{y}) := \frac{n}{2} \left( \frac{1}{2} + \frac{1}{y} \right) \sum_i \min\{x_i, y_i\}\]

Shared Nearest Neighbor Similarity Function \text{(since 0.1)}
de.lmu.ifi.dbs.elki.distance.similarityfunction.\text{SharedNearestNeighborSimilarityFunction}
SharedNearestNeighborSimilarityFunction with a pattern defined to accept Strings that define a non-negative Integer.

F.2.1 Cluster
de.lmu.ifi.dbs.elki.distance.similarityfunction.\text{cluster} \text{package:}
Similarity measures for comparing clusters.
Cluster Intersection Similarity Function  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.cluster.ClusterIntersectionSimilarityFunction}  
(since 0.7.0)  
Measure the similarity of clusters via the intersection size.

Cluster Jaccard Similarity Function  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.cluster.ClusterJaccardSimilarityFunction}  
(since 0.7.0)  
Measure the similarity of clusters via the Jaccard coefficient.

Clustering Adjusted Rand Index Similarity Function  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.cluster.ClusteringAdjustedRandIndexSimilarityFunction}  
(since 0.7.0)  
Measure the similarity of clusters via the Adjusted Rand Index.

Clustering B Cubed F1 Similarity Function  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.cluster.ClusteringBCubedF1SimilarityFunction}  
(since 0.7.0)  
Measure the similarity of clusters via the BCubed F1 Index.

Clustering Fowlkes Mallows Similarity Function  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.cluster.ClusteringFowlkesMallowsSimilarityFunction}  
(since 0.7.0)  
Measure the similarity of clusters via the Fowlkes-Mallows Index.

Clustering Rand Index Similarity Function  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.cluster.ClusteringRandIndexSimilarityFunction}  
(since 0.7.0)  
Measure the similarity of clusters via the Rand Index.

F.2.2 Kernel  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.kernel} package:  
Kernel functions.

Laplace Kernel Function  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.kernel.LaplaceKernelFunction}  
(since 0.6.0)  
Laplace / exponential radial basis function kernel.

Linear Kernel Function  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.kernel.LinearKernelFunction}  
(since 0.1)  
Linear Kernel function that computes a similarity between the two feature vectors \(x\) and \(y\) defined by \(x^T \cdot y\).

Note: this is effectively equivalent to using \texttt{EuclideanDistanceFunction}

Polynomial Kernel Function  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.kernel.PolynomialKernelFunction}  
(since 0.1)  
Polynomial Kernel function that computes a similarity between the two feature vectors \(x\) and \(y\) defined by \((x^T \cdot y + b)^\text{degree}\).

Radial Basis Function Kernel Function  
\texttt{de.lmu.ifi.dbs.elki.distance.similarityfunction.kernel.RadialBasisFunctionKernelFunction}  
(since 0.6.0)  
Gaussian radial basis function kernel (RBF Kernel).
Rational Quadratic Kernel Function
(de.lmu.ifi.dbs.elki.distance.similarityfunction.kernel.RationalQuadraticKernelFunction)
Rational quadratic kernel, a less computational approximation of the Gaussian RBF kernel (RadialBasisFunctionKernelFunction).

Sigmoid Kernel Function
(de.lmu.ifi.dbs.elki.distance.similarityfunction.kernel.SigmoidKernelFunction)
Sigmoid kernel function (aka: hyperbolic tangent kernel, multilayer perceptron MLP kernel).

G Evaluation
(de.lmu.ifi.dbs.elki.evaluation package:
Functionality for the evaluation of algorithms.

G.1 Classification
(de.lmu.ifi.dbs.elki.evaluation.classification package:
Evaluation of classification algorithms.

G.1.1 Holdout
(de.lmu.ifi.dbs.elki.evaluation.classification.holdout package:
Holdout and cross-validation strategies for evaluating classifiers.

Disjoint Cross Validation
(de.lmu.ifi.dbs.elki.evaluation.classification.holdout.DisjointCrossValidation)
DisjointCrossValidationHoldout provides a set of partitions of a database to perform cross-validation. The test sets are guaranteed to be disjoint.

Leave One Out
(de.lmu.ifi.dbs.elki.evaluation.classification.holdout.LeaveOneOut)
A leave-one-out-holdout is to provide a set of partitions of a database where each instances once hold out as a test instance while the respectively remaining instances are training instances.

Randomized Cross Validation
(de.lmu.ifi.dbs.elki.evaluation.classification.holdout.RandomizedCrossValidation)
RandomizedCrossValidationHoldout provides a set of partitions of a database to perform cross-validation. The test sets are not guaranteed to be disjoint.

Stratified Cross Validation
(de.lmu.ifi.dbs.elki.evaluation.classification.holdout.StratifiedCrossValidation)
A stratified n-fold crossvalidation to distribute the data to n buckets where each bucket exhibits approximately the same distribution of classes as does the complete data set. The buckets are disjoint. The distribution is deterministic.

G.2 Clustering
(de.lmu.ifi.dbs.elki.evaluation.clustering package:
Evaluation of clustering results.

B Cubed
(de.lmu.ifi.dbs.elki.evaluation.clustering.BCubed)
BCubed measures.
**Edit Distance**

Edit distance measures.

P. Pantel, D. Lin
Document clustering with committees
Proc. 25th ACM SIGIR Conf. on Research and Development in Information Retrieval

**Entropy**

Entropy based measures.

**Evaluate Clustering**

Evaluate a clustering result by comparing it to an existing cluster label.

**Log Cluster Sizes**

This class will log simple statistics on the clusters detected, such as the cluster sizes and the number of clusters.

**Pair Counting**

Pair-counting measures.

**Set Matching Purity**

Set matching purity measures.

**Extractor**

Classes to extract clusterings from hierarchical clustering.

**Cut Dendrogram By Height Extractor**

Extract clusters from a hierarchical clustering, during the evaluation phase. Usually, it is more elegant to use ExtractFlatClusteringFromHierarchy as primary algorithm. But in order to extract multiple partitionings from the same clustering, this can be useful.

**Cut Dendrogram By Number Of Clusters Extractor**

Extract clusters from a hierarchical clustering, during the evaluation phase. Usually, it is more elegant to use ExtractFlatClusteringFromHierarchy as primary algorithm. But in order to extract multiple partitionings from the same clustering, this can be useful.

**HDBSCAN Hierarchy Extraction Evaluator**

Extract clusters from a hierarchical clustering, during the evaluation phase. Usually, it is more elegant to use HDBSCANHierarchyExtraction as primary algorithm. But in order to extract multiple partitionings from the same clustering, this can be useful.
Simplified Hierarchy Extraction Evaluator (since 0.7.0)
de.lmu.ifi.dbs.elki.evaluation.clustering.extractor.SimplifiedHierarchyExtractionEvaluator

Extract clusters from a hierarchical clustering, during the evaluation phase. Usually, it is more elegant to use SimplifiedHierarchyExtraction as primary algorithm. But in order to extract multiple partitionings from the same clustering, this can be useful.

G.2.2 Internal
de.lmu.ifi.dbs.elki.evaluation.clustering.internal package:
Internal evaluation measures for clusterings.

Evaluate C Index (since 0.7.0)
de.lmu.ifi.dbs.elki.evaluation.clustering.internal.EvaluateCIndex
Compute the C-index of a data set.
Note: This requires pairwise distance computations, so it is not recommended to use this on larger data sets.

Evaluate Concordant Pairs (BH75, Roh74) (since 0.7.0)
de.lmu.ifi.dbs.elki.evaluation.clustering.internal.EvaluateConcordantPairs
Compute the Gamma Criterion of a data set.

Evaluate DBCV (MJC+14) (since 0.7.5)
de.lmu.ifi.dbs.elki.evaluation.clustering.internal.EvaluateDBCV
Compute the Density-Based Clustering Validation Index.

Evaluate Davies Bouldin (DB79) (since 0.7.0)
de.lmu.ifi.dbs.elki.evaluation.clustering.internal.EvaluateDaviesBouldin
Compute the Davies-Bouldin index of a data set.

Evaluate PBM Index (PBM04) (since 0.7.0)
de.lmu.ifi.dbs.elki.evaluation.clustering.internal.EvaluatePBMIndex
Compute the PBM index of a clustering

Evaluate Silhouette (Rou87) (since 0.7.0)
de.lmu.ifi.dbs.elki.evaluation.clustering.internal.EvaluateSilhouette
Compute the silhouette of a data set.

Evaluate Simplified Silhouette (since 0.7.0)
de.lmu.ifi.dbs.elki.evaluation.clustering.internal.EvaluateSimplifiedSilhouette
Compute the simplified silhouette of a data set.
The simplified silhouette does not use pairwise distances, but distances to centroids only.

Evaluate Squared Errors (since 0.7.0)
de.lmu.ifi.dbs.elki.evaluation.clustering.internal.EvaluateSquaredErrors
Evaluate a clustering by reporting the squared errors (SSE, SSQ), as used by k-means. This should be used with SquaredEuclideanDistanceFunction only (when used with other distances, it will manually square the values; but beware that the result is less meaningful with other distance functions).
For clusterings that provide a cluster prototype object (e.g. k-means), the prototype will be used. For other algorithms, the centroid will be recomputed.
Evaluate Variance Ratio Criteria (since 0.7.0)

de.lmu.ifi.dbs.elki.evaluation.clustering.internal.EvaluateVarianceRatioCriteria

Compute the Variance Ratio Criteria of a data set, also known as Calinski-Harabasz index.

G.2.3 Pairsegments

de.lmu.ifi.dbs.elki.evaluation.clustering.pairsegments package:

Pair-segment analysis of multiple clusterings.

Cluster Pair Segment Analysis (since 0.5.0)

de.lmu.ifi.dbs.elki.evaluation.clustering.pairsegments.ClusterPairSegmentAnalysis

Evaluate clustering results by building segments for their pairs: shared pairs and differences.

Segments (since 0.5.0)

de.lmu.ifi.dbs.elki.evaluation.clustering.pairsegments Segments

Creates segments of two or more clusterings.

Segments are the equally paired database objects of all given (2+) clusterings. Given a contingency table, an object Segment represents the table's cells where an intersection of classes and labels are given. Pair Segments are created by converting an object Segment into its pair representation. Converting all object Segments into pair Segments results in a larger number of pair Segments, if any fragmentation (no perfect match of clusters) within the contingency table has occurred (multiple cells on one row or column). Thus for ever object Segment exists a corresponding pair Segment. Additionally pair Segments represent pairs that are only in one Clustering which occurs for each split of a clusterings cluster by another clustering. Here, these pair Segments are referenced as fragmented Segments. Within the visualization they describe (at least two) pair Segments that have a corresponding object Segment.

G.3 Outlier

de.lmu.ifi.dbs.elki.evaluation.outlier package:

Evaluate an outlier score using a misclassification based cost model.

Compute Outlier Histogram (since 0.3)

de.lmu.ifi.dbs.elki.evaluation.outlier ComputeOutlierHistogram

Compute a Histogram to evaluate a ranking algorithm.

The parameter -hist.positive specifies the class label of "positive" hits.

Judge Outlier Scores (since 0.4.0)

de.lmu.ifi.dbs.elki.evaluation.outlier JudgeOutlierScores

Compute a Histogram to evaluate a ranking algorithm.

The parameter -hist.positive specifies the class label of "positive" hits.

Outlier Precision At K Curve (since 0.5.0)

de.lmu.ifi.dbs.elki.evaluation.outlier OutlierPrecisionAtKCurve

Compute a curve containing the precision values for an outlier detection method.

Outlier Precision Recall Curve (since 0.5.0)

de.lmu.ifi.dbs.elki.evaluation.outlier OutlierPrecisionRecallCurve

Compute a curve containing the precision values for an outlier detection method.

Outlier ROC Curve (since 0.2)

de.lmu.ifi.dbs.elki.evaluation.outlier OutlierROCCurve

Compute a ROC curve to evaluate a ranking algorithm and compute the corresponding ROCAUC value.
The parameter `-rocauc.positive` specifies the class label of “positive” hits. The nested algorithm `-algorithm` will be run, the result will be searched for an iterable or ordering result, which then is compared with the clustering obtained via the given class label.

**Outlier Ranking Evaluation** *(since 0.7.0)*
de.lmu.ifi.dbs.elki.evaluation.outlier.OutlierRankingEvaluation
Evaluate outlier scores by their ranking.

**Outlier Sm ROC Curve** *(since 0.5.0)*
de.lmu.ifi.dbs.elki.evaluation.outlier.OutlierSmROCCurve
Smooth ROC curves are a variation of classic ROC curves that takes the scores into account.

**Outlier Threshold Clustering** *(since 0.5.0)*
de.lmu.ifi.dbs.elki.evaluation.outlier.OutlierThresholdClustering
Pseudo clustering algorithm that builds clusters based on their outlier score. Useful for transforming a numeric outlier score into a 2-class dataset.

**G.4 Scores**
de.lmu.ifi.dbs.elki.evaluation.scores package:
Evaluation of rankings and scorings.

**Average Precision Evaluation** *(since 0.7.0)*
de.lmu.ifi.dbs.elki.evaluation.scores.AveragePrecisionEvaluation
Evaluate using average precision.

**DCG Evaluation** *(since 0.7.5)*
de.lmu.ifi.dbs.elki.evaluation.scores.DCGEvaluation
Discounted Cumulative Gain.
This evaluation metric would be able to use relevance information, but the current implementation is for binary labels only (it is easy to add, but requires API additions or changes).

**Maximum F1 Evaluation** *(since 0.7.0)*
de.lmu.ifi.dbs.elki.evaluation.scores.MaximumF1Evaluation
Evaluate using the maximum F1 score.

**NDCG Evaluation** *(since 0.7.5)*
de.lmu.ifi.dbs.elki.evaluation.scores.NDCGEvaluation
Normalized Discounted Cumulative Gain.
This evaluation metric would be able to use relevance information, but the current implementation is for binary labels only (it is easy to add, but requires API additions or changes).

**Precision At K Evaluation** *(since 0.7.0)*
de.lmu.ifi.dbs.elki.evaluation.scores.PrecisionAtKEvaluation
Evaluate using Precision@k, or R-precision (when k=0).
When k=0, then it is set to the number of positive objects, and the returned value is the R-precision, or the precision-recall break-even-point (BEP).

**ROC Evaluation** *(since 0.7.0)*
de.lmu.ifi.dbs.elki.evaluation.scores.ROCEvaluation
Compute ROC (Receiver Operating Characteristics) curves.
A ROC curve compares the true positive rate (y-axis) and false positive rate (x-axis).
It was first used in radio signal detection, but has since found widespread use in information retrieval, in particular for evaluating binary classification problems.

ROC curves are particularly useful to evaluate a ranking of objects with respect to a binary classification problem: a random sampling will approximately achieve a ROC value of 0.5, while a perfect separation will achieve 1.0 (all positives first) or 0.0 (all negatives first). In most use cases, a score significantly below 0.5 indicates that the algorithm result has been used the wrong way, and should be used backwards.

G.5 Similaritymatrix

de.lmu.ifi.dbs.elki.evaluation.similaritymatrix package:
Render a distance matrix to visualize a clustering-distance-combination.

Compute Similarity Matrix Image (since 0.4.0)
de.lmu.ifi.dbs.elki.evaluation.similaritymatrix.ComputeSimilarityMatrixImage
Compute a similarity matrix for a distance function.

H Index

de.lmu.ifi.dbs.elki.index package:
Index structure implementations

H.1 Distancematrix

de.lmu.ifi.dbs.elki.index.distancematrix package:
Precomputed distance matrix.

Precomputed Distance Matrix (since 0.7.0)
de.lmu.ifi.dbs.elki.index.distancematrix.PrecomputedDistanceMatrix
Distance matrix, for precomputing similarity for a small data set.
This class uses a linear memory layout (not a ragged array), and assumes symmetry as well as strictness. This way, it only stores the upper triangle matrix with double precision. It has to store \((n-1)\times(n-2)\) distance values in memory, requiring \(8\times(n-1)\times(n-2)\) bytes. Since Java has a size limit of arrays of 31 bits (signed integer), we can store at most \(2^{16}\) objects (precisely, 65536 objects) in a single array, which needs about 16 GB of RAM.

Precomputed Similarity Matrix (since 0.7.0)
de.lmu.ifi.dbs.elki.index.distancematrix.PrecomputedSimilarityMatrix
Precomputed similarity matrix, for a small data set.
This class uses a linear memory layout (not a ragged array), and assumes symmetry as well as strictness. This way, it only stores the upper triangle matrix with double precision. It has to store \((n-1)\times(n-2)\) similarity values in memory, requiring \(8\times(n-1)\times(n-2)\) bytes. Since Java has a size limit of arrays of 31 bits (signed integer), we can store at most \(2^{16}\) objects (precisely, 65536 objects) in a single array, which needs about 16 GB of RAM.

H.2 Idistance

de.lmu.ifi.dbs.elki.index.idistance package:
iDistance is a distance based indexing technique, using a reference points embedding.

In Memory I Distance Index (YOTJ01 JOT+05) (since 0.7.0)
de.lmu.ifi.dbs.elki.index.idistance.InMemoryIDistanceIndex
In-memory iDistance index, a metric indexing method using a reference point embedding.
Important note: we are currently using a different query strategy. The original publication discusses queries based on repeated radius queries. We use a strategy based on shrinking spheres, iteratively refined starting with the closest reference point. We also do not use a B+-tree as data structure, but simple in-memory lists. Therefore, we cannot report page accesses needed.

Feel free to contribute improved query strategies. All the code is essentially here, you only need to query every reference point list, not just the best.

H.3 Invertedlist

de.lmu.ifi.dbs.elki.index.invertedlist package:
Indexes using inverted lists.

In Memory Inverted Index

de.lmu.ifi.dbs.elki.index.invertedlist.InMemoryInvertedIndex
Simple index using inverted lists.

H.4 Lsh

de.lmu.ifi.dbs.elki.index.lsh package:
Locality Sensitive Hashing

In Memory LSH Index

de.lmu.ifi.dbs.elki.index.lsh.InMemoryLSHIndex
Locality Sensitive Hashing.

H.4.1 Hashfamilies

de.lmu.ifi.dbs.elki.index.lsh.hashfamilies package:
Hash function families for LSH.

Cosine Hash Function Family

de.lmu.ifi.dbs.elki.index.lsh.hashfamilies.CosineHashFunctionFamily
Hash function family to use with Cosine distance, using simplified hash functions where the projection is only drawn from +1, instead of Gaussian distributions.

Euclidean Hash Function Family

de.lmu.ifi.dbs.elki.index.lsh.hashfamilies.EuclideanHashFunctionFamily
2-stable hash function family for Euclidean distances.

Manhattan Hash Function Family

de.lmu.ifi.dbs.elki.index.lsh.hashfamilies.ManhattanHashFunctionFamily
2-stable hash function family for Euclidean distances.

H.4.2 Hashfunctions

de.lmu.ifi.dbs.elki.index.lsh.hashfunctions package:
Hash functions for LSH.

Cosine Locality Sensitive Hash Function

de.lmu.ifi.dbs.elki.index.lsh.hashfunctions.CosineLocalitySensitiveHashFunction
Random projection family to use with sparse vectors.
Multiple Projections Locality Sensitive Hash Function \cite{DIM04} (since 0.6.0)
de.lmu.ifi.dbs.elki.index.lsh.hashfunctions.MultipleProjectionsLocalitySensitiveHashFunction
LSH hash function for vector space data. Depending on the choice of random vectors, it can be appropriate for Manhattan and Euclidean distances.

H.5 Preprocessed

de.lmu.ifi.dbs.elki.index.preprocessed package:
Index structure based on preprocessors

H.5.1 Fastoptics

de.lmu.ifi.dbs.elki.index.preprocessed.fastoptics package:
Preprocessed index used by the FastOPTICS algorithm.

Random Projected Neighbors And Densities \cite{SV13} (since 0.7.0)
de.lmu.ifi.dbs.elki.index.preprocessed.fastoptics.RandomProjectedNeighborsAndDensities
Random Projections used for computing neighbors and density estimates.
This index is specialized for the algorithm FastOPTICS

H.5.2 Knn

de.lmu.ifi.dbs.elki.index.preprocessed.knn package:
Indexes providing KNN and rKNN data.

NN Descent \cite{DCL11} (since 0.7.5)
de.lmu.ifi.dbs.elki.index.preprocessed.knn.NNDescent
NN-desent (also known as KNNGraph) is an approximate nearest neighbor search algorithm beginning with a random sample, then iteratively refining this sample until.

Spacefilling KNN Preprocessor \cite{SZK15} (since 0.7.0)
de.lmu.ifi.dbs.elki.index.preprocessed.knn.SpacefillingKNNPreprocessor
Compute the nearest neighbors approximatively using space filling curves.
This version computes the data projections and stores, then queries this data on-demand. This usually needs less memory (except for very small neighborhood sizes k) than SpacefillingMaterializeKNNPreprocessor, but will also be slower.

Spacefilling Materialize KNN Preprocessor \cite{SZK15} (since 0.7.0)
de.lmu.ifi.dbs.elki.index.preprocessed.knn.SpacefillingMaterializeKNNPreprocessor
Compute the nearest neighbors approximatively using space filling curves.
This version does the bulk kNN-join operation, i.e. precomputes the k nearest neighbors for every object, then discards the curves. This is usually more memory intensive but faster than SpacefillingKNNPreprocessor.

H.5.3 Localpca

de.lmu.ifi.dbs.elki.index.preprocessed.localpca package:
Index using a preprocessed local PCA.

Knn Query Based Local PCA Preprocessor (since 0.4.0)
de.lmu.ifi.dbs.elki.index.preprocessed.localpca.KNNQueryFilteredPCAIIndex
Provides the local neighborhood to be considered in the PCA as the k nearest neighbors of an object.
H.5.4 Preference

Indexes storing preference vectors.

DiSH Preference Vector Index

Preprocessor for DiSH preference vector assignment to objects of a certain database.

HiSC Preprocessor

Preprocessor for HiSC preference vector assignment to objects of a certain database.

H.5.5 Snn

Indexes providing nearest neighbor sets

Shared Nearest Neighbor Preprocessor

A preprocessor for annotation of the ids of nearest neighbors to each database object.
This functionality is similar but not identical to MaterializeKNNPreprocessor: While it also computes
the k nearest neighbors, it does not keep the actual distances, but organizes the NN set in a TreeSet for fast
set operations.

H.6 Projected

Projected indexes for data.

LatLngAsECEF Index

Index a 2d data set (consisting of Lat/Lng pairs) by using a projection to 3D coordinates (WGS-86 to ECEF).
Earth-Centered, Earth-Fixed (ECEF) is a 3D coordinate system, sometimes also referred to as XYZ, that
uses 3 cartesian axes. The center is at the earths center of mass, the z axis points to the north pole. X axis
is to the prime meridian at the equator (so latitude 0, longitude 0), and the Y axis is orthogonal going to the
east (latitude 0, longitude 90°E).
The Euclidean distance in this coordinate system is a lower bound for the great-circle distance, and
Euclidean coordinates are supposedly easier to index.
Note: this index will only support the distance function LatLngDistanceFunction, as it uses a projection
that will map data according to this great circle distance. If the query hint "exact" is set, it will not be used.

LngLatAsECEF Index

Index a 2d data set (consisting of Lng/Lat pairs) by using a projection to 3D coordinates (WGS-86 to ECEF).
Earth-Centered, Earth-Fixed (ECEF) is a 3D coordinate system, sometimes also referred to as XYZ, that
uses 3 cartesian axes. The center is at the earths center of mass, the z axis points to the north pole. X axis
is to the prime meridian at the equator (so latitude 0, longitude 0), and the Y axis is orthogonal going to the
east (latitude 0, longitude 90°E).
The Euclidean distance in this coordinate system is a lower bound for the great-circle distance, and
Euclidean coordinates are supposedly easier to index.
Note: this index will only support the distance function LngLatDistanceFunction, as it uses a projection
that will map data according to this great circle distance. If the query hint "exact" is set, it will not be used.
PINN: Projection Indexed Nearest Neighbors \[\text{dvCH10} \text{ (since 0.6.0)}\]
d&e.letmu.ifi.dbs.elki.index.projected\PINN

Projection-Indexed nearest-neighbors (PINN) is an index to retrieve the nearest neighbors in high dimensional spaces by using a random projection based index.

H.7 Tree
d&e.letmu.ifi.dbs.elki.index.tree package:
Tree-based index structures

H.7.1 Metrical
d&e.letmu.ifi.dbs.elki.index.tree.metrical package:
Tree-based index structures for metrical vector spaces.

Metrical Covertree d&e.letmu.ifi.dbs.elki.index.tree.metrical.covertree package:
Cover-tree variations.

Cover Tree \[\text{BKL06} \text{ (since 0.7.0)}\]
d&e.letmu.ifi.dbs.elki.index.tree.metrical.covertree.CoverTree
Cover tree data structure (in-memory). This is a metrical data structure that is similar to the M-tree, but not as balanced and disk-oriented. However, by not having these requirements it does not require the expensive splitting procedures of M-tree.

Simplified Cover Tree \(\text{ (since 0.7.0)}\)
d&e.letmu.ifi.dbs.elki.index.tree.metrical.covertree.SimplifiedCoverTree
Simplified cover tree data structure (in-memory). This is a metrical data structure that is similar to the M-tree, but not as balanced and disk-oriented. However, by not having these requirements it does not require the expensive splitting procedures of M-tree. This version does not store the distance to the parent, so it needs only about 40% of the memory of CoverTree but does more distance computations for search.

Metrical Mtreevariants d&e.letmu.ifi.dbs.elki.index.tree.metrical.mtreevariants package:
M-Tree and variants.

Metrical Mtreevariants Mktrees d&e.letmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.mktrees package:
Metrical index structures based on the concepts of the M-Tree supporting processing of reverse k nearest neighbor queries by using the k-nn distances of the entries.

Metrical Mtreevariants Mktrees Mkapp d&e.letmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.mktrees.mkapp package:
MkAppTree

MkApp Tree Factory \(\text{(since 0.4.0)}\)
d&e.letmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.mktrees.mkapp.MkAppTreeFactory
Factory for a MkApp-Tree

Metrical Mtreevariants Mktrees Mkmax d&e.letmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.mktrees.mkmax package:
MkMaxTree
MkMax Tree Factory (since 0.4.0)
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.mktrees.mkmax.MkMaxTreeFactory
Factory for MkMaxTrees

Metrical Mtreevariants Mktab
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.mktrees.mktab
package:
MkTabTree

MkTab Tree Factory (since 0.4.0)
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.mktrees.mktab.MkTabTreeFactory
Factory for MkTabTrees

Metrical Mtreevariants Mtree
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.mtree
package:
MTree

M-Tree [CPZ97] (since 0.1)
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.mtree.MTree
MTree is a metrical index structure based on the concepts of the M-Tree. Apart from organizing the objects it also provides several methods to search for certain object in the structure. Persistence is not yet ensured.

M Tree Factory (since 0.4.0)
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.mtree.MTreeFactory
Factory for a M-Tree

Metrical Mtreevariants Strategies
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.strategies
package:

Metrical Mtreevariants Strategies Insert
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.strategies.insert
package:
Insertion (choose path) strategies of nodes in an M-Tree (and variants).

Minimum Enlargement Insert [CPZ97] (since 0.6.0)
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.strategies.insert.MinimumEnlargementInsert
Minimum enlargement insert - default insertion strategy for the M-tree.

Metrical Mtreevariants Strategies Split
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.strategies.split
package:
Splitting strategies of nodes in an M-Tree (and variants).

Farthest Points Split (since 0.7.5)
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.strategies.split.FarthestPointsSplit
Farthest points split.

MLB Dist Split [CPZ97] (since 0.6.0)
de.lmu.ifi.dbs.elki.index.tree.metrical.mtreevariants.strategies.split.MLBDistSplit
Encapsulates the required methods for a split of a node in an M-Tree. The routing objects are chosen according to the MLBDIST strategy. The benefit of this strategy is that it works with precomputed distances from the parent, while most other strategies would require $O(n^2)$ distance computations. So if construction time is critical, this is a good choice.
MMRad Split
Encapsulates the required methods for a split of a node in an M-Tree. The routing objects are chosen according to the mMrad strategy.

MRad Split
Encapsulates the required methods for a split of a node in an M-Tree. The routing objects are chosen according to the Mrad strategy.

MST Split
Splitting algorithm using the minimum spanning tree (MST), as proposed by the Slim-Tree variant.
Unfortunately, the slim-tree paper does not detail how to choose the "most appropriate edge from the longest ones" (to find a more balanced split), so we try to longest 50%, and keep the choice which yields the most balanced split. This seems to work quite well.

Random Split
Encapsulates the required methods for a split of a node in an M-Tree. The routing objects are chosen according to the RANDOM strategy.
Note: only the routing objects are chosen at random, this is not a random assignment!

Balanced Distribution
Balanced entry distribution strategy of the M-tree.

Farthest Balanced Distribution
Balanced entry distribution strategy of the M-tree, beginning with the most difficult points first. This should produce smaller covers.

Generalized Hyperplane Distribution
Generalized hyperplane entry distribution strategy of the M-tree.
This strategy does not produce balanced trees, but often produces faster access times, according to the original publication.

H.7.2 Spatial
Tree-based index structures for spatial indexing.

Spatial Kd
K-d-tree and variants.
Minimalistic Memory KD Tree

Simple implementation of a static in-memory K-D-tree. Does not support dynamic updates or anything, but also is very simple and memory efficient: all it uses is one ArrayModifiableDBIDs to sort the data in a serialized tree.

Small Memory KD Tree

Simple implementation of a static in-memory K-D-tree. Does not support dynamic updates or anything, but also is very simple and memory efficient: all it uses is one ModifiableDoubleDBIDList to sort the data in a serialized tree and store the current attribute value.

It needs about 3 times as much memory as MinimalisticMemoryKDTree but it is also considerably faster because it does not need to lookup this value from the vectors.

Spatial Rstarvariants

R*-Tree and variants.

Spatial Rstarvariants Query

Queries on the R-Tree family of indexes: kNN and range queries.

Euclidean R Star Tree KNN Query

Instance of a KNN query for a particular spatial index.

Euclidean R Star Tree Range Query

Instance of a range query for a particular spatial index.

R Star Tree KNN Query

Instance of a KNN query for a particular spatial index.

R Star Tree Range Query

Instance of a range query for a particular spatial index.

Spatial Rstarvariants Rstar

RStarTree

R*-Tree

RStarTree is a spatial index structure based on the concepts of the R*-Tree. Apart from organizing the objects it also provides several methods to search for certain object in the structure and ensures persistence.

R Star Tree Factory

Factory for regular R*-Trees.

Spatial Rstarvariants Strategies

strategies package:
Spatial Rstarvariants Strategies Bulk  de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.bulk package:
Packages for bulk-loading R*-Trees.

Adaptive Sort Tile Recursive Bulk Split
(de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.bulk.AdaptiveSortTileRecursiveBulkSplit)
This is variation of the original STR bulk load for non-rectangular data spaces. Instead of iterating through the dimensions and splitting each by (approximately) the same factor, this variation tries to adjust the factor to the extends of the data space. I.e. if the data set is twice as wide as high, this should produce twice as many partitions on the X than on the Y axis.
Whether or not this offers benefits greatly depends on the distance queries used. But for symmetric distances, the resulting pages should be more rectangular, which often is beneficial. See SortTileRecursiveBulkSplit for the original STR bulk load.

File Order Bulk Split
(de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.bulk.FileOrderBulkSplit)
Trivial bulk loading - assumes that the file has been appropriately sorted before.

Max Extension Bulk Split
(de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.bulk.MaxExtensionBulkSplit)
Split strategy for bulk-loading a spatial tree where the split axes are the dimensions with maximum extension.

Max Extension Sort Tile Recursive Bulk Split
(de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.bulk.MaxExtensionSortTileRecursiveBulkSplit)
This is variation of the SortTileRecursiveBulkSplit, incorporating some ideas from MaxExtensionBulkSplit. Instead of iterating through the axes in order, it always chooses the axis with the largest extend. This may rarely lead to the data being split on the same axis twice, but most importantly it varies the splitting order compared to STR.
AdaptiveSortTileRecursiveBulkSplit takes these ideas one step further, by also varying the fan-out degree.

OneDim Sort Bulk Split
(de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.bulk.OneDimSortBulkSplit)
Simple bulk loading strategy by sorting the data along the first dimension.
This is also known as Nearest-X, and attributed to:
N. Roussopoulos, D. Leifker
Direct spatial search on pictorial databases using packed R-trees
ACM SIGMOD Record 14-4

Sort Tile Recursive Bulk Split
(de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.bulk.SortTileRecursiveBulkSplit)
Sort-Tile-Recursive aims at tiling the data space with a grid-like structure for partitioning the dataset into the required number of buckets.

Spatial Sort Bulk Split
(de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.bulk.SpatialSortBulkSplit)
Bulk loading by spatially sorting the objects, then partitioning the sorted list appropriately.
Based conceptually on:
On packing R-trees
I. Kamel, C. Faloutsos
Proc. 2nd Int. Conf. on Information and Knowledge Management (CIKM)

Spatial Rstarvariants Strategies Insert
Insertion strategies for R-Trees

Approximative Least Overlap Insertion Strategy [BKSS90] (since 0.5.0)
The choose subtree method proposed by the R*-Tree with slightly better performance for large leaf sizes (linear approximation).
Norbert Beckmann, Hans-Peter Kriegel, Ralf Schneider, Bernhard Seeger
The R*-tree: an efficient and robust access method for points and rectangles
Proc. 1990 ACM SIGMOD Int. Conf. Management of Data

Combined Insertion Strategy [BKSS90] (since 0.5.0)
Use two different insertion strategies for directory and leaf nodes.
Norbert Beckmann, Hans-Peter Kriegel, Ralf Schneider, Bernhard Seeger
The R*-tree: an efficient and robust access method for points and rectangles
Proc. 1990 ACM SIGMOD Int. Conf. Management of Data

Least Enlargement Insertion Strategy [Gut84] (since 0.5.0)
The default R-Tree insertion strategy: find rectangle with least volume enlargement.

Least Enlargement With Area Insertion Strategy [BKSS90] (since 0.5.0)
A slight modification of the default R-Tree insertion strategy: find rectangle with least volume enlargement, but choose least area on ties.
Proposed for non-leaf entries in:
Norbert Beckmann, Hans-Peter Kriegel, Ralf Schneider, Bernhard Seeger
The R*-tree: an efficient and robust access method for points and rectangles
Proc. 1990 ACM SIGMOD Int. Conf. Management of Data

Least Overlap Insertion Strategy [BKSS90] (since 0.5.0)
The choose subtree method proposed by the R*-Tree for leaf nodes.

Spatial Rstarvariants Strategies Overflow
Overflow treatment strategies for R-Trees
**Limited Reinsert Overflow Treatment**  
**(BKSS90) (since 0.5.0)**

de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.overflow.LimitedReinsertOverflowTreatment

Limited reinsertions, as proposed by the R*-Tree: For each real insert, allow reinsertions to happen only once per level.

**Split Only Overflow Treatment**  
**(since 0.5.0)**

de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.overflow.SplitOnlyOverflowTreatment

Always split, as in the original R-Tree

**Spatial Rstarvariants Strategies Reinsert**  
de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.reinsert package:

Reinsertion strategies for R-Trees

**Close Reinsert**  
**(BKSS90) (since 0.5.0)**

de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.reinsert.CloseReinsert

Reinsert objects on page overflow, starting with close objects first (even when they will likely be inserted into the same page again!)

The strategy preferred by the R*-Tree

**Far Reinsert**  
**(BKSS90) (since 0.5.0)**

de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.reinsert.FarReinsert

Reinsert objects on page overflow, starting with farther objects first (even when they will likely be inserted into the same page again!)

Alternative strategy mentioned in the R*-tree

**Spatial Rstarvariants Strategies Split**  
de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.split package:

Splitting strategies for R-Trees

**AngTan Linear Split**  
**(AT97) (since 0.5.0)**

de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.split.AngTanLinearSplit

Line-time complexity split proposed by Ang and Tan.

This split strategy tries to minimize overlap only, which can however degenerate to "slices".

**Greene Split**  
**(Gre89) (since 0.5.0)**

de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.split.GreeneSplit

Quadratic-time complexity split as used by Diane Greene for the R-Tree.

Seed selection is quadratic, distribution is O(n log n).

This contains a slight modification to improve performance with point data: with points as seeds, the normalized separation is always 1, so we choose the raw separation then.

D. Greene

An implementation and performance analysis of spatial data access methods

Proceedings of the Fifth International Conference on Data Engineering

**R Tree Linear Split**  
**(Gut84) (since 0.5.0)**

de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.split.RTreeLinearSplit

Linear-time complexity greedy split as used by the original R-Tree.
R Tree Quadratic Split  \[\text{Gut84}\] (since 0.5.0)
de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.split.RTreeQuadraticSplit
Quadratic-time complexity greedy split as used by the original R-Tree.

Topological Splitter  \[\text{BKSS90}\] (since 0.4.0)
de.lmu.ifi.dbs.elki.index.tree.spatial.rstarvariants.strategies.split.TopologicalSplitter
Encapsulates the required parameters for a topological split of a R*-Tree.

H.8 Vafie

Vector Approximation File

delmu.ifi.dbs.elki.index.vafie package:

DA File  \[\text{KKSZ06}\] (since 0.5.0)
de.lmu.ifi.dbs.elki.index.vafie.DAFile
Dimension approximation file, a one-dimensional part of the PartialVAFile.

Partial VA File  \[\text{KKSZ06}\] (since 0.5.0)
de.lmu.ifi.dbs.elki.index.vafie.PartialVAFile
PartialVAFile. In-memory only implementation.

An approximation based data structure for similarity search  \[\text{WB97}\] (since 0.5.0)
de.lmu.ifi.dbs.elki.index.vafie.VAFile
Vector-approximation file (VAFile)

I Math

Mathematical operations and utilities used throughout the framework.

Mean  \[\text{Nee66}\] (since 0.2)
de.lmu.ifi.dbs.elki.math.Mean
Compute the mean using a numerically stable online algorithm.
This class can repeatedly be fed with data using the put() methods, the resulting values for mean can be queried at any time using getMean().
The high-precision function is based on:
P. M. Neely
Comparison of Several Algorithms for Computation of Means, Standard Deviations and Correlation Coefficients
Communications of the ACM 9(7), 1966

Mean Variance  \[\text{Wel62, SG18b, YC71, Wes79}\] (since 0.2)
de.lmu.ifi.dbs.elki.math.MeanVariance
Do some simple statistics (mean, variance) using a numerically stable online algorithm.
This class can repeatedly be fed with data using the add() methods, the resulting values for mean and average can be queried at any time using Mean.getMean() and getSampleVariance().
Make sure you have understood variance correctly when using getNaiveVariance() - since this class is fed with samples and estimates the mean from the samples, getSampleVariance() is often the more appropriate version.
As experimentally studied in

86
Erich Schubert, Michael Gertz
Numerically Stable Parallel Computation of (Co-)Variance
Proc. 30th Int. Conf. Scientific and Statistical Database Management (SSDBM 2018)
the current approach is based on:
E. A. Youngs and E. M. Cramer
Some Results Relevant to Choice of Sum and Sum-of-Product Algorithms
Technometrics 13(3), 1971
We have originally experimented with:
B. P. Welford
Note on a method for calculating corrected sums of squares and products
Technometrics 4(3), 1962
D. H. D. West
Updating Mean and Variance Estimates: An Improved Method
Communications of the ACM 22(9)

Statistical Moments
[SG18b, YC71, Ter07, Pé08] (since 0.6.0)
delmu.ifi.dbs.elki.math.StatisticalMoments
Track various statistical moments, including mean, variance, skewness and kurtosis.

I.1 Geodesy

delmu.ifi.dbs.elki.math.geodesy package:
Functions for computing on the sphere / earth.

Clarke 1858 Spheroid Earth Model
[SG18b, YC71, Ter07, Pé08] (since 0.6.0)
delmu.ifi.dbs.elki.math.geodesy.Clarke1858SpheroidEarthModel
The Clarke 1858 spheroid earth model.
Radius: 6378293.645 m
Flattening: 1 / 294.26068

Clarke 1880 Spheroid Earth Model
[SG18b, YC71, Ter07, Pé08] (since 0.6.0)
delmu.ifi.dbs.elki.math.geodesy.Clarke1880SpheroidEarthModel
The Clarke 1880 spheroid earth model.
Radius: 6378249.145 m
Flattening: 1 / 293.465

GRS67 Spheroid Earth Model
[SG18b, YC71, Ter07, Pé08] (since 0.6.0)
delmu.ifi.dbs.elki.math.geodesy.GRS67SpheroidEarthModel
The GRS 67 spheroid earth model.
Radius: 6378160.0 m
Flattening: 1 / 298.25

GRS80 Spheroid Earth Model
[SG18b, YC71, Ter07, Pé08] (since 0.6.0)
delmu.ifi.dbs.elki.math.geodesy.GRS80SpheroidEarthModel
The GRS 80 spheroid earth model, without height model (so not a geoid, just a spheroid!)
Radius: 6378137.0 m
Flattening: 1 / 298.25

Sphere Util
[SZK13, Wil11, Vin75, Sin84] (since 0.5.5)
delmu.ifi.dbs.elki.math.geodesy.SphereUtil
Class with utility functions for distance computations on the sphere.
Note: the formulas are usually implemented for the unit sphere.
The majority of formulas are adapted from:
E. Williams
Aviation Formulary
Online: http://www.edwilliams.org/avform.htm

Spherical Cosine Earth Model (since 0.6.0)
de.lmu.ifi.dbs.elki.math.geodesy.SphericalCosineEarthModel
A simple spherical earth model using radius 6371009 m.
For distance computations, this variant uses the Cosine formula, which is faster but less accurate than the Haversine or Vincenty's formula.

Spherical Haversine Earth Model (since 0.6.0)
de.lmu.ifi.dbs.elki.math.geodesy.SphericalHaversineEarthModel
A simple spherical earth model using radius 6371009 m.
For distance computations, this variant uses the Haversine formula, which is faster but less accurate than Vincenty's formula.

Spherical Vincenty Earth Model (since 0.6.0)
de.lmu.ifi.dbs.elki.math.geodesy.SphericalVincentyEarthModel
A simple spherical earth model using radius 6371009 m.

WGS72 Spheroid Earth Model (since 0.6.0)
de.lmu.ifi.dbs.elki.math.geodesy.WGS72SpheroidEarthModel
The WGS72 spheroid earth model, without height model.
Radius: 6378135.0 m
Flattening: 1 / 298.26

WGS84 Spheroid Earth Model (since 0.6.0)
de.lmu.ifi.dbs.elki.math.geodesy.WGS84SpheroidEarthModel
The WGS84 spheroid earth model, without height model (so not a geoid, just a spheroid!)
Note that EGM96 uses the same spheroid, but what really makes the difference is its geoid expansion.
Radius: 6378137.0 m
Flattening: 1 / 298.257223563

I.2 Geometry

de.lmu.ifi.dbs.elki.math.geometry package:
Algorithms from computational geometry.

Graham Scan Convex Hull 2D (since 0.4.0)
de.lmu.ifi.dbs.elki.math.geometry.GrahamScanConvexHull2D
Classes to compute the convex hull of a set of points in 2D, using the classic Grahams scan. Also computes a bounding box.

Prims Minimum Spanning Tree (since 0.5.5)
de.lmu.ifi.dbs.elki.math.geometry.PrimsMinimumSpanningTree
Prim's algorithm for finding the minimum spanning tree.
Implementation for dense graphs, represented as distance matrix.

Sweep Hull Delaunay 2D (since 0.5.0)
de.lmu.ifi.dbs.elki.math.geometry.SweepHullDelaunay2D
Compute the Convex Hull and/or Delaunay Triangulation, using the sweep-hull approach of David Sinclair.
I.3 Linearalgebra

The linear algebra package provides classes and computational methods for operations on matrices and vectors.

Some content of this package is adapted from the Jama package.

Five fundamental matrix decompositions, which consist of pairs or triples of matrices, permutation vectors, and the like, produce results in five decomposition classes. These decompositions are accessed by the Matrix class to compute solutions of simultaneous linear equations, determinants, inverses and other matrix functions. The five decompositions are:

- Cholesky Decomposition of symmetric, positive definite matrices.
- LU Decomposition of rectangular matrices.
- QR Decomposition of rectangular matrices.
- Singular Value Decomposition of rectangular matrices.
- Eigenvalue Decomposition of both symmetric and nonsymmetric square matrices.

Example of use: Solve a linear system \( Ax = b \) and compute the residual norm, \( ||b - Ax|| \).

```java
double[][] matrix = {1., 2., 3., 4., 5., 6., 7., 8., 10.};
double[] b = MathUtil.randomDoubleArray(3, new Random());
double[] x = VMath.solve(matrix, b);
double[] r = VMath.minusEquals(VMath.times(matrix, x), b);
double norm = VMath.euclideanLength(r);
```

The original Jama-package has been developed by the MathWorks and NIST and can be found at math.nist.gov. Here, for the adaption some classes and methods convenient for data mining applications within ELKI were added. Furthermore some erroneous comments were corrected and the coding-style was subtly changed to a more Java-typical style.

Vector and Matrix Math Library [Mah36] (since 0.5.0)

Class providing basic vector mathematics, for low-level vectors stored as `double[]`. While this is less nice syntactically, it reduces memory usage and VM overhead.

I.3.1 Pca

Principal Component Analysis (PCA) and Eigenvector processing.

Autotuning PCA [KKSZ08] (since 0.5.0)

Performs a self-tuning local PCA based on the covariance matrices of given objects. At most the closest 'k' points are used in the calculation and a weight function is applied.

The number of points used depends on when the strong eigenvectors exhibit the clearest correlation.

PCA Runner (since 0.2)

Class to run PCA on given data.

The various methods will start PCA at different places (e.g. with database IDs, database query results, a precomputed covariance matrix or eigenvalue decomposition).

The runner can be parameterized by setting a covariance matrix builder (e.g. to a weighted covariance matrix builder)
RANSAC Covariance Matrix Builder

Since 0.5.5

de.lmu.ifi.dbs.elki.math.linearalgebra.pca.RANSAC Covariance Matrix Builder

RANSAC based approach to a more robust covariance matrix computation. This is an experimental adoption of RANSAC to this problem, not a generic RANSAC implementation! While using RANSAC for PCA at first sounds like a good idea, it does not work very well in high-dimensional spaces. The problem is that PCA has $O(n^2)$ degrees of freedom, so we need to sample very many objects, then perform an $O(n^3)$ matrix operation to compute PCA, for each attempt.

Standard Covariance Matrix Builder

Since 0.2

de.lmu.ifi.dbs.elki.math.linearalgebra.pca.Standard Covariance Matrix Builder

Class for building a "traditional" covariance matrix via CovarianceMatrix. Reasonable default choice for a CovarianceMatrixBuilder.

Weighted Covariance Matrix / PCA

Since 0.2

de.lmu.ifi.dbs.elki.math.linearalgebra.pca.Weighted Covariance Matrix Builder

CovarianceMatrixBuilder with weights. This builder uses a weight function to weight points differently during build a covariance matrix. Covariance can be canonically extended with weights, as shown in the article.

Pca Filter

de.lmu.ifi.dbs.elki.math.linearalgebra.pca.filter package:

Filter eigenvectors based on their eigenvalues.

Drop EigenPair Filter

Since 0.5.0

de.lmu.ifi.dbs.elki.math.linearalgebra.pca.filter.Drop EigenPair Filter

The "drop" filter looks for the largest drop in normalized relative eigenvalues. Let $s_1 \ldots s_n$ be the eigenvalues.

Let $a_k := 1/(n-k) \sum_{i=k..n} s_i$.

Then $r_k := s_k/a_k$ is the relative eigenvalue.

The drop filter searches for $\arg \max_k r_k/r_{k+1}$.

First n Eigenpair Filter

Since 0.1

de.lmu.ifi.dbs.elki.math.linearalgebra.pca.filter.First n Eigenpair Filter

The FirstNEigenPairFilter marks the $n$ highest eigenpairs as strong eigenpairs, where $n$ is a user specified number.

Limit-based Eigenpair Filter

Since 0.1

de.lmu.ifi.dbs.elki.math.linearalgebra.pca.filter.Limit EigenPair Filter

The LimitEigenPairFilter marks all eigenpairs having an (absolute) eigenvalue below the specified threshold (relative or absolute) as weak eigenpairs, the others are marked as strong eigenpairs.

Percentage based Eigenpair Filter

Since 0.1

de.lmu.ifi.dbs.elki.math.linearalgebra.pca.filter.Percentage EigenPair Filter

The PercentageEigenPairFilter sorts the eigenpairs in descending order of their eigenvalues and marks the first eigenpairs, whose sum of eigenvalues is higher than the given percentage of the sum of all eigenvalues as strong eigenpairs.

Progressive Eigenpair Filter

Since 0.2

de.lmu.ifi.dbs.elki.math.linearalgebra.pca.filter.Progressive EigenPair Filter

The ProgressiveEigenPairFilter sorts the eigenpairs in descending order of their eigenvalues and marks the first eigenpairs, whose sum of eigenvalues is higher than the given percentage of the sum of all eigenvalues as strong eigenpairs. In contrast to the PercentageEigenPairFilter, it will use a percentage which changes linearly with the subspace dimensionality. This makes the parameter more consistent for
different dimensionalities and often gives better results when clusters of different dimensionality exist, since different percentage alpha levels might be appropriate for different dimensionalities.

Example calculations of alpha levels:

In a 3D space, a progressive alpha value of 0.5 equals:
- 1D subspace: 50% + 1/3 of remainder = 0.667
- 2D subspace: 50% + 2/3 of remainder = 0.833

In a 4D space, a progressive alpha value of 0.5 equals:
- 1D subspace: 50% + 1/4 of remainder = 0.625
- 2D subspace: 50% + 2/4 of remainder = 0.750
- 3D subspace: 50% + 3/4 of remainder = 0.875

Reasoning why this improves over PercentageEigenPairFilter:
In a 100 dimensional space, a single Eigenvector representing over 85% of the total variance is highly significant, whereas the strongest 85 Eigenvectors together will by definition always represent at least 85% of the variance. PercentageEigenPairFilter can thus not be used with these parameters and detect both dimensionalities correctly.

The second parameter introduced here, walpha, serves a different function: It prevents the eigenpair filter to use a statistically weak Eigenvalue just to reach the intended level, e.g. 84% + 1% >= 85% when 1% is statistically very weak.

Relative EigenPair Filter

The RelativeEigenPairFilter sorts the eigenpairs in descending order of their eigenvalues and marks the first eigenpairs who are a certain factor above the average of the remaining eigenvalues.

It is closely related to the WeakEigenPairFilter, and differs mostly by comparing to the remaining Eigenvalues, not to the total sum.

There are some situations where one or the other is superior, especially when it comes to handling nested clusters and strong global correlations that are not too interesting. These benefits usually only make a difference at higher dimensionalities.

Significant EigenPair Filter

The SignificantEigenPairFilter sorts the eigenpairs in descending order of their eigenvalues and chooses the contrast of an Eigenvalue to the remaining Eigenvalues is maximal.

It is closely related to the WeakEigenPairFilter and RelativeEigenPairFilter. But while the RelativeEigenPairFilter chooses the highest dimensionality that satisfies the relative alpha levels, the SignificantEigenPairFilter will chose the local dimensionality such that the 'contrast' is maximal.

There are some situations where one or the other is superior, especially when it comes to handling nested clusters and strong global correlations that are not too interesting. These benefits usually only make a difference at higher dimensionalities.

Weak Eigenpair Filter

The WeakEigenPairFilter sorts the eigenpairs in descending order of their eigenvalues and returns the first eigenpairs who are above the average mark as 'strong', the others as 'weak'.

Pca Weightfunctions

Weight functions used in weighted PCA via WeightedCovarianceMatrixBuilder

Constant Weight

The result is always 1.0
**Erfc Stddev Weight**  
(de.lmu.ifi.dbs.elki.math.linearalgebra.pca.weightfunctions.ErfcStddevWeight)  
Gaussian Error Function Weight function, scaled using stddev. This probably is the most statistically sound weight.  
\[ \text{erfc}(1 / \sqrt{2} \cdot \text{distance} / \text{stddev}) \]

**Erfc Weight**  
(de.lmu.ifi.dbs.elki.math.linearalgebra.pca.weightfunctions.ErfcWeight)  
Gaussian Error Function Weight function, scaled such that the result is 0.1 at distance == max  
\[ \text{erfc}(1.1630871536766736 \cdot \text{distance} / \text{max}) \]  
The value of 1.1630871536766736 is \( \text{erfc}^{-1}(0.1) \), to achieve the intended scaling.

**Exponential Stddev Weight**  
(de.lmu.ifi.dbs.elki.math.linearalgebra.pca.weightfunctions.ExponentialStddevWeight)  
Exponential Weight function, scaled such that the result is 0.1 at distance == max  
\[ \text{stddev} \cdot \exp(-0.5 \cdot \text{distance} / \text{stddev}) \]  
This is similar to the Gaussian weight function, except distance/stddev is not squared.

**Exponential Weight**  
(de.lmu.ifi.dbs.elki.math.linearalgebra.pca.weightfunctions.ExponentialWeight)  
Exponential Weight function, scaled such that the result is 0.1 at distance == max  
\[ \exp(-2.3025850929940455 \cdot \text{distance} / \text{max}) \]  
This is similar to the Gaussian weight function, except distance/max is not squared. -2.3025850929940455 is \( \log(-0.1) \) to achieve the intended range of 1.0 - 0.1

**Gauss Stddev Weight**  
(de.lmu.ifi.dbs.elki.math.linearalgebra.pca.weightfunctions.GaussStddevWeight)  
Gaussian weight function, scaled using standard deviation  
\[ \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\text{dist}^2}{2\sigma^2}\right) \]

**Gauss Weight**  
(de.lmu.ifi.dbs.elki.math.linearalgebra.pca.weightfunctions.GaussWeight)  
Gaussian weight function, scaled such that the result is 0.1 at distance == max, using  
\[ \exp(-2.3025850929940455 \cdot \frac{\text{dist}^2}{\text{max}^2}) \]

**Inverse Linear Weight**  
(de.lmu.ifi.dbs.elki.math.linearalgebra.pca.weightfunctions.InverseLinearWeight)  
Inverse Linear Weight Function.  
This weight is not particularly reasonable. Instead it serves the purpose of testing the effects of a badly chosen weight function.  
This function has increasing weight, from 0.1 to 1.0 at distance == max.

**Inverse Proportional Stddev Weight**  
(de.lmu.ifi.dbs.elki.math.linearalgebra.pca.weightfunctions.InverseProportionalStddevWeight)  
Inverse proportional weight function, scaled using the standard deviation.  
\[ 1 / (1 + \text{distance} / \text{stddev}) \]

**Inverse Proportional Weight**  
(de.lmu.ifi.dbs.elki.math.linearalgebra.pca.weightfunctions.InverseProportionalWeight)  
Inverse proportional weight function, scaled using the maximum.  
\[ 1 / (1 + \text{distance} / \text{max}) \]
Linear Weight

Linear weight function, scaled using the maximum such that it goes from 1.0 to 0.1
\[ 1 - 0.9 \times \left( \frac{\text{distance}}{\max} \right) \]

Quadratic Stddev Weight

Quadratic weight function, scaled using the standard deviation.
We needed another scaling here, we chose the cutoff point to be \(3\sigma\). If you need another value, you have to reimplement this class.
\[ \max\{0.0, 1.0 - \frac{\text{dist}^2}{3\sigma^2}\} \]

Quadratic Weight

Quadratic weight function, scaled using the maximum to reach 0.1 at that point.
\[ 1.0 - 0.9 \times \left( \frac{\text{distance}}{\max} \right)^2 \]

I.4 Spacefillingcurves

Space filling curves.

Binary Split Spatial Sorter

Spatially sort the data set by repetitive binary splitting, circulating through the dimensions. This is essentially the bulk-loading proposed for the k-d-tree, as it will produce a perfectly balanced k-d-tree. The resulting order is the sequence in which objects would then be stored in the k-d-tree.
Note that when using this for bulk-loading an R-tree, the result will not be a k-d-tree, not even remotely similar, as the splits are not preserved.

Hilbert Spatial Sorter

Sort object along the Hilbert Space Filling curve by mapping them to their Hilbert numbers and sorting them.
Objects are mapped using 31 bits per dimension.

Peano Spatial Sorter

Bulk-load an R-tree index by presorting the objects with their position on the Peano curve.
The basic shape of this space-filling curve looks like this:

```
3---4
|   |
2 5 8
|   |
1   6---7
```
Which then expands to the next level as:

```
+-+-+-+-+-+- E
|   |   |   |   |
|   |   |   |   |
|   |   |   |   |
|   |   |   |   |
|   |   |   |   |
```

and so on.

**Z Curve Spatial Sorter**  
*ZCurveSpatialSorter*  
Class to sort the data set by their Z-index, without doing a full materialization of the Z indexes.

### I.5 Statistics

**Probability Weighted Moments**  
*ProbabilityWeightedMoments*  
Estimate the L-Moments of a sample.

#### I.5.1 Dependence

**Correlation Dependence Measure**  
*CorrelationDependenceMeasure*  
Pearson product-moment correlation coefficient.

**Distance Correlation Dependence Measure**  
*DistanceCorrelationDependenceMeasure*  
Distance correlation. The value returned is the square root of the dCor² value. This matches the R implementation by the original authors.

**HSM Dependence Measure**  
*HSMDependenceMeasure*  
Compute the 'interestingness' of dimension connections using the hough transformation. This is a very visual approach, designed to find certain patterns in parallel coordinates visualizations. The patterns detected here occur mostly if you have multiple clusters of linear patterns as far as we understood the approach (which is not easy to use, unfortunately).

**HiCS Dependence Measure**  
*HiCSDependenceMeasure*  
Use the statistical tests as used by HiCS to measure dependence of variables.

**Hoeffdings D Dependence Measure**  
*HoeffdingsDDependenceMeasure*  
Calculate Hoeffding’s D as a measure of dependence.

**Jensen Shannon Equiwidth Dependence Measure**  
*JensenShannonEquiwidthDependenceMeasure*  
Jensen-Shannon Divergence is closely related to mutual information. The output value is normalized, such that an evenly distributed and identical distribution will yield a value of 1. Independent distributions may still yield values close to .25, though.
MCE Dependence Measure  
\cite{Guo03} (since 0.7.0)
de.lmu.ifi.dbs.elki.math.statistics.dependence.MCEDependenceMeasure
Compute a mutual information based dependence measure using a nested means discretization, originally proposed for ordering axes in parallel coordinate plots.

Mutual Information Equiwidth Dependence Measure
\cite{Guo03} (since 0.7.0)
de.lmu.ifi.dbs.elki.math.statistics.dependence.MutualInformationEquiwidthDependenceMeasure
Mutual Information (MI) dependence measure by dividing each attribute into equal-width bins. MI can be seen as Kullback–Leibler divergence of the joint distribution and the product of the marginal distributions. For normalization, the resulting values are scaled by $\frac{mi}{\log(nbins)}$. This both cancels out the logarithm base, and normalizes for the number of bins (a uniform distribution will yield a MI with itself of 1).

SURFING Dependence Measure \cite{AKSZ13, BPK+04} (since 0.5.5)
de.lmu.ifi.dbs.elki.math.statistics.dependence.SURFINGDependenceMeasure
Compute the similarity of dimensions using the SURFING score. The parameter $k$ for the $k$ nearest neighbors is currently hard-coded to 10% of the set size.
Note that the complexity is roughly $O(n n k)$, so this is a rather slow method, and with $k$ at 10% of $n$, is actually cubic: $O(0.1 n^2)$.
This version cannot use index support, as the API operates without database attachment. However, it should be possible to implement some trivial sorted-list indexes to get a reasonable speedup!

Slope Dependence Measure \cite{AKSZ13} (since 0.5.5)
de.lmu.ifi.dbs.elki.math.statistics.dependence.SlopeDependenceMeasure
Arrange dimensions based on the entropy of the slope spectrum.
This version only accepts positive correlations, see also SlopeInversionDependenceMeasure.

Slope Inversion Dependence Measure \cite{AKSZ13} (since 0.5.5)
de.lmu.ifi.dbs.elki.math.statistics.dependence.SlopeInversionDependenceMeasure
Arrange dimensions based on the entropy of the slope spectrum.

Spearman Correlation Dependence Measure
\cite{Guo03} (since 0.7.0)
de.lmu.ifi.dbs.elki.math.statistics.dependence.SpearmanCorrelationDependenceMeasure
Spearman rank-correlation coefficient, also known as Spearman’s Rho.

I.5.2 Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution package:
Standard distributions, with random generation functionalities.

Beta Distribution
\cite{Guo03} (since 0.5.0)
de.lmu.ifi.dbs.elki.math.statistics.distribution.BetaDistribution
Beta Distribution with implementation of the regularized incomplete beta function

Cauchy Distribution
\cite{Guo03} (since 0.6.0)
de.lmu.ifi.dbs.elki.math.statistics.distribution.CauchyDistribution
Cauchy distribution.

Chi Distribution
\cite{Guo03} (since 0.5.0)
de.lmu.ifi.dbs.elki.math.statistics.distribution.ChiDistribution
Chi distribution.
Chi Squared Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.ChiSquaredDistribution

Chi-Squared distribution (a specialization of the Gamma distribution).

Constant Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.ConstantDistribution

Pseudo distribution, that has a unique constant value.

Exp Gamma Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.ExpGammaDistribution

Exp-Gamma Distribution, with random generation and density functions.

This distribution can be outlined as Y log\[\Gamma\] distributed, or equivalently \(\exp(Y)\) Gamma.

Note: this matches the loggamma of SciPy, whereas Wolfram calls this the Exponential Gamma Distribution "at times confused with the LogGammaDistribution".

Exponential Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.ExponentialDistribution

Exponential distribution.

Exponentially Modified Gaussian Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.ExponentiallyModifiedGaussianDistribution

Exponentially modified Gaussian (EMG) distribution (ExGaussian distribution) is a combination of a normal distribution and an exponential distribution.

Note that scipy uses a subtly different parameterization.

Gamma Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.GammaDistribution

Gamma Distribution, with random generation and density functions.

Generalized Extreme Value Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.GeneralizedExtremeValueDistribution

Generalized Extreme Value (GEV) distribution, also known as Fisher–Tippett distribution.

This is a generalization of the Frechhet, Gumbel and (reversed) Weibull distributions.

Implementation notice: In ELKI 0.8.0, the sign of the shape was negated.

Generalized Logistic Alternate Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.GeneralizedLogisticAlternateDistribution

Generalized logistic distribution.

One of multiple ways of generalizing the logistic distribution.

Where \(\text{shape}=0\) yields the regular logistic distribution.

Generalized Logistic Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.GeneralizedLogisticDistribution

Generalized logistic distribution. (Type I, Skew-logistic distribution)

One of multiple ways of generalizing the logistic distribution.

\[
pdf(x) = \text{shape} \times \exp(-x) / (1 + \exp(-x))^{(\text{shape}+1)}
\]

\[
cdf(x) = \text{pow}(1+\exp(-x), -\text{shape})
\]

Where \(\text{shape}=1\) yields the regular logistic distribution.
Generalized Pareto Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.GeneralizedParetoDistribution

Generalized Pareto Distribution (GPD), popular for modeling long tail distributions.

Gumbel Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.GumbelDistribution

Gumbel distribution, also known as Log-Weibull distribution.

Halton Uniform Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.HaltonUniformDistribution

Halton sequences are a pseudo-uniform distribution. The data is actually too regular for a true uniform
distribution, but as such will of course often appear to be uniform.

Technically, they are based on Van der Corput sequence and the Von Neumann Katutani transformation.
These produce a series of integers which then are converted to floating point values.

To randomize, we just choose a random starting position, as indicated by

Inverse Gaussian Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.InverseGaussianDistribution

Inverse Gaussian distribution aka Wald distribution.

Beware that SciPy uses a different location parameter.

InverseGaussian(a, x) scipy.stats.invgauss(a/x, x) Our parameter scheme is in line with
common literature. SciPy naming scheme has comparable notion of location and scale across distributions.
So both have their benefits.

Kappa Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.KappaDistribution

Kappa distribution, by Hosking.

Laplace Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.LaplaceDistribution

Laplace distribution also known as double exponential distribution

Log Gamma Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.LogGammaDistribution

Log-Gamma Distribution, with random generation and density functions.

This distribution can be outlined as Y exp(Gamma) or equivalently Log(Y) Gamma.

Note: this is a different loggamma than scipy uses, but corresponds to the Log Gamma Distribution of
Wolfram, who notes that it is “at times confused with ExpGammaDistribution”.

Log Logistic Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.LogLogisticDistribution

Log-Logistic distribution also known as Fisk distribution.

Log Normal Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.LogNormalDistribution

Log-Normal distribution.

The parameterization of this class is somewhere inbetween of GNU R and SciPy. Similar to GNU R we use
the logmean and logstddev. Similar to Scipy, we also have a location parameter that shifts the distribution.
Our implementation maps to SciPy’s as follows: scipy.stats.lognorm(logstddev, shift, Fast-
Math.exp(logmean))
Logistic Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.LogisticDistribution

Logistic distribution.

Normal Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.NormalDistribution

Gaussian distribution aka normal distribution

Poisson Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.PoissonDistribution

INCOMPLETE implementation of the poisson distribution.

Rayleigh Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.RayleighDistribution

Rayleigh distribution, a special case of the Weibull distribution.

Skew Generalized Normal Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.SkewGeneralizedNormalDistribution

Generalized normal distribution by adding a skew term, similar to lognormal distributions. This is one kind of generalized normal distributions. Note that there are multiple that go by the name of a "Generalized Normal Distribution"; this is what is currently called "version 2" in English Wikipedia.

Students T Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.StudentsTDistribution

Student's t distribution.

Uniform Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.UniformDistribution

Uniform distribution.

Weibull Distribution

de.lmu.ifi.dbs.elki.math.statistics.distribution.WeibullDistribution

Weibull distribution.

Distribution Estimator

de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator package: Estimators for statistical distributions.

Cauchy MAD Estimator

de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.CauchyMADEstimator

Estimate Cauchy distribution parameters using Median and MAD.

EMG Olivier Norberg Estimator

de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.EMGOlivierNorbergEstimator

Naive distribution estimation using mean and sample variance.

Exp Gamma Exp MOM Estimator

de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.ExpGammaExpMOMEstimator

Simple parameter estimation for the ExpGamma distribution. This is a very naive estimation, based on the mean and variance only, sometimes referred to as the "Method of Moments" (MOM). This estimator based on the GammaMOMEstimator and a simple exp data transformation.
Exponential LMM Estimator

Estimate the parameters of a Gamma Distribution, using the methods of L-Moments (LMM).

Exponential MAD Estimator

Estimate Exponential distribution parameters using Median and MAD.

Exponential MOM Estimator

Estimate Exponential distribution parameters using the mean, which is the maximum-likelihood estimate (MLE), but not very robust.

Exponential Median Estimator

Estimate Exponential distribution parameters using Median and MAD.

Gamma Choi Wette Estimator

Estimate distribution parameters using the method by Choi and Wette.

Gamma LMM Estimator

Estimate the parameters of a Gamma Distribution, using the methods of L-Moments (LMM).

Gamma MOM Estimator

Simple parameter estimation for the Gamma distribution.

This is a very naive estimation, based on the mean and variance only, sometimes referred to as the "Method of Moments" (MOM).

Generalized Extreme Value LMM Estimator

Estimate the parameters of a Generalized Extreme Value Distribution, using the methods of L-Moments (LMM).

Generalized Logistic Alternate LMM Estimator

Estimate the parameters of a Generalized Logistic Distribution, using the methods of L-Moments (LMM).

Generalized Pareto LMM Estimator

Estimate the parameters of a Generalized Pareto Distribution (GPD), using the methods of L-Moments (LMM).
Gumbel LMM Estimator
\[ \text{(since 0.6.0)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.GumbelLMMEstimator} 
Estimate the parameters of a Gumbel Distribution, using the methods of L-Moments (LMM).

Gumbel MAD Estimator
\[ \text{(since 0.6.0)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.GumbelMADEstimator} 
Parameter estimation via median and median absolute deviation from median (MAD).

Inverse Gaussian ML Estimator
\[ \text{(since 0.6.0)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.InverseGaussianMLEstimator} 
Estimate parameter of the inverse Gaussian (Wald) distribution.

Inverse Gaussian MOM Estimator
\[ \text{(since 0.6.0)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.InverseGaussianMOMEstimator} 
Estimate parameter of the inverse Gaussian (Wald) distribution.

Laplace LMM Estimator
\[ \text{(since 0.6.0)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.LaplaceLMMEstimator} 
Estimate Laplace distribution parameters using the method of L-Moments (LMM).

Laplace MAD Estimator
\[ \text{(since 0.6.0)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.LaplaceMADEstimator} 
Estimate Laplace distribution parameters using Median and MAD.

Laplace MLE Estimator
\[ \text{(since 0.6.0)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.LaplaceMLEEstimator} 
Estimate Laplace distribution parameters using Median and mean deviation from median.

Log Gamma Log MOM Estimator
\[ \text{(since 0.7.5)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.LogGammaLogMOMEstimator} 
Simple parameter estimation for the LogGamma distribution.
This is a very naive estimation, based on the mean and variance only, sometimes referred to as the "Method of Moments" (MOM).
This estimator based on the GammaMOMEstimator and a simple log data transformation.

Log Logistic MAD Estimator
\[ \text{(since 0.6.0)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.LogLogisticMADEstimator} 
Estimate Logistic distribution parameters using Median and MAD.

Log Normal Bilkova LMM Estimator
\[ \text{(since 0.6.0)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.LogNormalBilkovaLMMEstimator} 
Alternate estimate the parameters of a log Gamma Distribution, using the methods of L-Moments (LMM) for the Generalized Normal Distribution.

Log Normal LMM Estimator
\[ \text{(since 0.6.0)} \]
\text{de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.LogNormalLMMEstimator} 
Estimate the parameters of a log Normal Distribution, using the methods of L-Moments (LMM) for the Generalized Normal Distribution.
Log Normal Levenberg Marquardt KDE Estimator
since 0.6.0
Distribution parameter estimation using Levenberg-Marquardt iterative optimization and a kernel density estimation.
Note: this estimator is rather expensive, and needs optimization in the KDE phase, which currently is O(n^3)!
This estimator is primarily attractive when only part of the distribution was observed.

Log Normal Log MAD Estimator [Ham74] (since 0.6.0)
Estimator using Medians. More robust to outliers, and just slightly more expensive (needs to copy the data for partial sorting to find the median).

Log Normal Log MOM Estimator (since 0.6.0)
Naive distribution estimation using mean and sample variance.
This is a maximum-likelihood-estimator (MLE).

Logistic LMM Estimator [Hos00] (since 0.6.0)
Estimate the parameters of a Logistic Distribution, using the methods of L-Moments (LMM).

Logistic MAD Estimator [Oli06] (since 0.6.0)
Estimate Logistic distribution parameters using Median and MAD.

Normal LMM Estimator [Hos00] (since 0.6.0)
Estimate the parameters of a normal distribution using the method of L-Moments (LMM).

Normal Levenberg Marquardt KDE Estimator (since 0.6.0)
Distribution parameter estimation using Levenberg-Marquardt iterative optimization and a kernel density estimation.
Note: this estimator is rather expensive, and needs optimization in the KDE phase, which currently is O(n^3)!
This estimator is primarily attractive when only part of the distribution was observed.

Normal MAD Estimator [Ham74] (since 0.6.0)
Estimator using Medians. More robust to outliers, and just slightly more expensive (needs to copy the data for partial sorting to find the median).

Normal MOM Estimator (since 0.6.0)
Naive maximum-likelihood estimations for the normal distribution using mean and sample variance.
While this is the most commonly used estimator, it is not very robust against extreme values.
Rayleigh LMM Estimator

delmuifi.dbs.elki.math.statistics.distribution.estimator.RayleighLMMEstimator
Estimate the scale parameter of a (non-shifted) RayleighDistribution using the method of L-Moments (LMM).

Rayleigh MAD Estimator

delmuifi.dbs.elki.math.statistics.distribution.estimator.RayleighMADEstimator
Estimate the parameters of a RayleighDistribution using the MAD.

Rayleigh MLE Estimator

delmuifi.dbs.elki.math.statistics.distribution.estimator.RayleighMLEEstimator
Estimate the scale parameter of a (non-shifted) RayleighDistribution using a maximum likelihood estimate.

Skew G Normal LMM Estimator

delmuifi.dbs.elki.math.statistics.distribution.estimator.SkewGNormalLMMEstimator
Estimate the parameters of a skew Normal Distribution (Hoskin’s Generalized Normal Distribution), using the methods of L-Moments (LMM).

Uniform Enhanced Min Max Estimator

delmuifi.dbs.elki.math.statistics.distribution.estimator.UniformEnhancedMinMaxEstimator
Slightly improved estimation, that takes sample size into account and enhances the interval appropriately.

Uniform LMM Estimator

delmuifi.dbs.elki.math.statistics.distribution.estimator.UniformLMMEstimator
Estimate the parameters of a normal distribution using the method of L-Moments (LMM).

Uniform MAD Estimator

delmuifi.dbs.elki.math.statistics.distribution.estimator.UniformMADEstimator
Estimate Uniform distribution parameters using Median and MAD.

Uniform Min Max Estimator

delmuifi.dbs.elki.math.statistics.distribution.estimator.UniformMinMaxEstimator
Estimate the uniform distribution by computing min and max.

Weibull LMM Estimator

delmuifi.dbs.elki.math.statistics.distribution.estimator.WeibullLMMEstimator
Estimate parameters of the Weibull distribution using the method of L-Moments (LMM).

Weibull Log MAD Estimator

delmuifi.dbs.elki.math.statistics.distribution.estimator.WeibullLogMADEstimator
Parameter estimation via median and median absolute deviation from median (MAD).

Distribution Estimator Meta
delmuifi.dbs.elki.math.statistics.distribution.estimator.meta
Meta estimators: estimators that do not actually estimate themselves, but instead use other estimators, e.g. on a trimmed data set, or as an ensemble.

Best Fit Estimator
delmuifi.dbs.elki.math.statistics.distribution.estimator.meta.BestFitEstimator
A meta estimator that will try a number of (inexpensive) estimations, then choose whichever works best.
Trimmed Estimator *(since 0.6.0)*
de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.meta.TrimmedEstimator
Trimmed wrapper around other estimators. Sorts the data, trims it, then analyzes it using another estimator.

Winsorizing Estimator *(HMTW47) (since 0.6.0)*
de.lmu.ifi.dbs.elki.math.statistics.distribution.estimator.meta.WinsorizingEstimator
Winsorizing or Georgization estimator. Similar to trimming, this is supposed to be more robust to outliers. However, instead of removing the extreme values, they are instead replaced with the cutoff value. This keeps the quantity of the data the same, and will have a lower impact on variance and similar measures.

### I.5.3 Intrinsic dimensionality

Methods for estimating the intrinsic dimensionality.

| Estimator                  | Reference   | Since       | Description                                                                 |
|----------------------------|-------------|-------------|-----------------------------------------------------------------------------|
| ALID Estimator             | [CHK16]     | 0.7.5       | ALID estimator of the intrinsic dimensionality (maximum likelihood estimator for ID using auxiliary distances). |
| Aggregated Hill Estimator  | [HKKP01]    | 0.7.0       | Estimator using the weighted average of multiple hill estimators.           |
| Ensemble Estimator         |             | 0.7.0       | Ensemble estimator taking the median of three of our best estimators.      |
|                           |             |             | However, the method-of-moments estimator seems to work best at least on artificial distances - you don’t benefit from always choosing the second best, so this ensemble approach does not appear to help. This is an experimental estimator. Please cite ELKI when using. |
| GED Estimator              | [HKN12]     | 0.7.0       | Generalized Expansion Dimension for estimating the intrinsic dimensionality. |
| Hill Estimator             | [Hil75]     | 0.7.0       | Hill estimator of the intrinsic dimensionality (maximum likelihood estimator for ID). |
| L Moments Estimator        | [Host00]    |             | Probability weighted moments based estimator using L-Moments.              |
|                           | [ACF+15]    |             | This is derived from the PWM estimators of Amsaleg et al. using the L-Moments estimation for the exponential distribution. |
| MOM Estimator              | [ACF+15]    |             | Methods of moments estimator, using the first moment (i.e. average).       |
|                           |             |             | This could be generalized to higher order moments, but the variance increases with the order, and we need this to work well with small sample sizes. |
PWM2 Estimator
[ACF+15 MMW79] (since 0.7.0)
delmu.ifi.dbs.elki.math.statistics.intrinsicdimensionality.PWM2Estimator
Probability weighted moments based estimator, using the second moment. It can be shown theoretically that this estimator is expected to have a higher variance than the one using the first moment only, it is included for completeness only.

PWM Estimator
[ACF+15 MMW79] (since 0.7.0)
delmu.ifi.dbs.elki.math.statistics.intrinsicdimensionality.PWMEstimator
Probability weighted moments based estimator.

RV Estimator
[ACF+15] (since 0.7.0)
delmu.ifi.dbs.elki.math.statistics.intrinsicdimensionality.RVEstimator
Regularly Varying Functions estimator of the intrinsic dimensionality

Zipf Estimator
[BDG05 SS96 KR96] (since 0.7.0)
delmu.ifi.dbs.elki.math.statistics.intrinsicdimensionality.ZipfEstimator
Zipf estimator (qq-estimator) of the intrinsic dimensionality. Unfortunately, this estimator appears to have a bias. We have empirically modified the plot position such that bias is reduced, but could not find the proper way of removing this bias for small samples.

I.5.4 Kernel functions

delmu.ifi.dbs.elki.math.statistics.kernelfunctions package: Kernel functions from statistics.

Biweight Kernel Density Function
[MN88] (since 0.6.0)
delmu.ifi.dbs.elki.math.statistics.kernelfunctions.BiweightKernelDensityFunction
Biweight (Quartic) kernel density estimator.

Cosine Kernel Density Function
(since 0.6.0)
delmu.ifi.dbs.elki.math.statistics.kernelfunctions.CosineKernelDensityFunction
Cosine kernel density estimator.

Epanechnikov Kernel Density Function
[MN88] (since 0.6.0)
delmu.ifi.dbs.elki.math.statistics.kernelfunctions.EpanechnikovKernelDensityFunction
Epanechnikov kernel density estimator.

Gaussian Kernel Density Function
[MN88] (since 0.6.0)
delmu.ifi.dbs.elki.math.statistics.kernelfunctions.GaussianKernelDensityFunction
Gaussian kernel density estimator.

Kernel Density Function
[MN88] (since 0.6.0)
delmu.ifi.dbs.elki.math.statistics.kernelfunctions.KernelDensityFunction
Inner function of a kernel density estimator.
Note: as of now, this API does not support asymmetric kernels, which would be difficult in the multivariate case.

Triangular Kernel Density Function
(since 0.6.0)
delmu.ifi.dbs.elki.math.statistics.kernelfunctions.TriangularKernelDensityFunction
Triangular kernel density estimator.
Tricube Kernel Density Function (since 0.6.0)
de.lmu.ifi.dbs.elki.math.statistics.kernelfunctions.TricubeKernelDensityFunction
Tricube kernel density estimator.

Triweight Kernel Density Function [MN88] (since 0.6.0)
de.lmu.ifi.dbs.elki.math.statistics.kernelfunctions.TriweightKernelDensityFunction
Triweight kernel density estimator.

Uniform Kernel Density Function [MN88] (since 0.6.0)
de.lmu.ifi.dbs.elki.math.statistics.kernelfunctions.UniformKernelDensityFunction
Uniform / Rectangular kernel density estimator.

I.5.5 Tests

de.lmu.ifi.dbs.elki.math.statistics.tests package:
Statistical tests.

Anderson Darling Test [AD52, Ste74] (since 0.7.0)
de.lmu.ifi.dbs.elki.math.statistics.tests.AndersonDarlingTest
Perform Anderson-Darling test for a Gaussian distribution.
This is a test against normality / goodness of fit. i.e. you can use it to reject the hypothesis that the data is
normal distributed. Such tests are sensitive to data set size: on small samples, even large deviations could
be by-chance and thus not allow rejection. On the other hand, on large data sets even a slight deviation
can be unlikely to happen if the data were indeed normal distributed. Thus, this test is more likely to fail
to reject small data sets even when they intuitively do not appear to be normal distributed, while it will
reject large data sets that originate from a distribution only slightly different from the normal distribution.
Before using, make sure you have understood statistical tests, and the difference between failure-to-reject
and acceptance!
The data size should be at least 8 before the results start getting somewhat reliable. For large data sets, the
chance of rejecting the normal distribution hypothesis increases a lot: no real data looks exactly like a
normal distribution.

Kolmogorov Smirnov Test (since 0.5.0)
de.lmu.ifi.dbs.elki.math.statistics.tests.KolmogorovSmirnovTest
Kolmogorov-Smirnov test.
Class that tests two given real-valued data samples on whether they might have originated from the same
underlying distribution using the Kolmogorov-Smirnov test statistic that compares the two empirical
cumulative distribution functions. The KS statistic is defined as the maximum absolute difference of the
empirical CDFs.

Standardized Two Sample Anderson Darling Test [Pet76, SS87, Dar57] (since 0.7.0)
de.lmu.ifi.dbs.elki.math.statistics.tests.StandardizedTwoSampleAndersonDarlingTest
Perform a two-sample Anderson-Darling rank test, and standardize the statistic according to Scholz and
Stephens. Ties are handled as discussed in Equation 7 of Scholz and Stephens.
To access the non-standardized A2 scores, use the function unstandardized(double[] []).n
Compared to the Cramer-van Mises test, the Anderson-Darling test puts more weight on the tail of the
distribution. This variant only uses the ranks.

Welch T Test (since 0.5.0)
de.lmu.ifi.dbs.elki.math.statistics.tests.WelchTTest
Calculates a test statistic according to Welch’s t test for two samples Supplies methods for calculating the
degrees of freedom according to the Welch-Satterthwaite Equation. Also directly calculates a two-sided
p-value for the underlying t-distribution
J Utilities

de.lmu.ifi.dbs.elki.utilities package:
Utility and helper classes - commonly used data structures, output formatting, exceptions, ...
Specialized utility classes (which often collect static utility methods only) can be found in other places of ELKI as well, as seen below.

Important utility function collections:
• Basic and low-level:
  - Util: Miscellaneous utility functions.
  - LoggingUtil: simple logging access.
  - MathUtil: Mathematics utility functions.
  - VectorUtil: Vector and Matrix functions.
  - SpatialUtil: Spatial MBR computations (intersection, union etc.).
  - ByteArrayUtil: byte array processing (low-level IO via byte arrays).
  - FileUtil: File and file name utility functions.
  - ClassGenericsUtil: Generic classes (instantiation, arrays of arrays, sets that require safe but unchecked casts).
• Database-related:
  - TypeUtil: Data type utility functions and common type definitions.
  - QueryUtil: Database Query API simplifications.
  - DBIDUtil: Database ID DBID handling.
  - DataStoreUtil: Data storage layer (like Maps).
  - DatabaseUtil: database utility functions (centroid etc.).
  - ResultUtil: result processing functions (e.g. extracting sub-results).
• Output-related:
  - FormatUtil: output formatting.
  - SVGUtil: SVG generation (XML DOM based).
  - BatikUtil: Apache Batik SVG utilities (coordinate transforms screen to canvas).
• Specialized:
  - OptionUtil: Managing parameter settings
  - ELKIServiceRegistry: class and classpath inspection.
  - RStarTreeUtil: reporting page file accesses.

J.1 Datastructures

de.lmu.ifi.dbs.elki.utilities.datastructures package:
Basic memory structures such as heaps and object hierarchies.

J.1.1 Arrays

de.lmu.ifi.dbs.elki.utilities.datastructures.arrays package:
Utilities for arrays: advanced sorting for primitive arrays.

Integer Array Quick Sort

delmu.ifi.dbs.elki.utilities.datastructures.arrays.IntegerArrayQuickSort
Class to sort an int array, using a modified quicksort.

J.1.2 Unionfind

de.lmu.ifi.dbs.elki.utilities.datastructures.unionfind package:
Union-find data structures.

Weighted Quick Union Integer

delmu.ifi.dbs.elki.utilities.datastructures.unionfind.WeightedQuickUnionInteger
Union-find algorithm for primitive integers, with optimizations. This is the weighted quick union approach, weighted by count and using path-halving for optimization.
Weighted Quick Union Range DBI Ds

Union-find algorithm for DBIDRange only, with optimizations.
To instantiate, use UnionFindUtil.make(de.lmu.ifi.dbs.elki.database.ids.StaticDBIDs).
This version is optimized for DBIDRanges.
This is the weighted quick union approach, weighted by count and using path-halving for optimization.

Weighted Quick Union Static DBI Ds

Union-find algorithm for StaticDBIDs, with optimizations.
To instantiate, use UnionFindUtil.make(de.lmu.ifi.dbs.elki.database.ids.StaticDBIDs),
which will automatically choose the best implementation available.
This is the weighted quick union approach, weighted by count and using path-halving for optimization.
This version needs more memory than WeightedQuickUnionRangeDBIDs but can work with any un-modifiable DBID set (although ArrayDBIDs are recommended).

J.2 Ensemble

Utility classes for simple ensembles.

Ensemble Voting Inverse Multiplicative

Inverse multiplicative voting: $1 - \prod_i (1 - s_i)$

Ensemble Voting Max

Simple combination rule, by taking the maximum.

Ensemble Voting Mean

Simple combination rule, by taking the mean

Ensemble Voting Median

Simple combination rule, by taking the median.
Note: median is very similar to a majority voting!

Ensemble Voting Min

Simple combination rule, by taking the minimum.

Ensemble Voting Multiplicative

Inverse multiplicative voting: $\prod_i s_i$

J.3 Random

Random number generation.
**Fast Non Threadsafe Random**

FastNonThreadsafeRandom (since 0.6.0)

Drop-in replacement for Random, but not using atomic long seeds. This implementation is no longer thread-safe (but faster)!

It is still the same Linear Congruential Generator (LCG), with a cycle length of $2^{48}$, of which we only use 32 bits at a time. Given the same seed, it is expected to produce the exact same random sequence as Java's Random.

**Xor Shift 1024 Non Threadsafe Random**

XorShift1024NonThreadsafeRandom (since 0.7.0)

Replacement for Java's Random class, using a different random number generation strategy. Java's random generator is optimized for speed, but may lack the randomness needed for more complex experiments.

This approach is based on the work on XorShift1024* by Sebastiano Vigna, with the original copyright statement:

Written in 2014 by Sebastiano Vigna (vigna@acm.org)

To the extent possible under law, the author has dedicated all copyright and related and neighboring rights to this software to the public domain worldwide. This software is distributed without any warranty.

See http://creativecommons.org/publicdomain/zero/1.0/

**Xor Shift 64 Non Threadsafe Random**

XorShift64NonThreadsafeRandom (since 0.7.0)

Replacement for Java's Random class, using a different random number generation strategy. Java's random generator is optimized for speed, but may lack the randomness needed for more complex experiments.

This approach is based on the work on XorShift64* by Sebastiano Vigna, with the original copyright statement:

Written in 2014 by Sebastiano Vigna (vigna@acm.org)

To the extent possible under law, the author has dedicated all copyright and related and neighboring rights to this software to the public domain worldwide. This software is distributed without any warranty.

See http://creativecommons.org/publicdomain/zero/1.0/

**Xoroshiro 128 Non Threadsafe Random**

Xoroshiro128NonThreadsafeRandom (since 0.7.5)

Replacement for Java's Random class, using a different random number generation strategy. Java's random generator is optimized for speed, but may lack the randomness needed for more complex experiments.

This approach is based on the work on Xoroshiro128+ by Sebastiano Vigna, with the original copyright statement:

Written in 2016 by David Blackman and Sebastiano Vigna (vigna@acm.org)

To the extent possible under law, the author has dedicated all copyright and related and neighboring rights to this software to the public domain worldwide. This software is distributed without any warranty.

See http://creativecommons.org/publicdomain/zero/1.0/

---

### J.4 Referencepoints

Referencepoints package:

Package containing strategies to obtain reference points

Shared code for various algorithms that use reference points.

**Axis Based Reference Points**

AxisBasedReferencePoints (since 0.3)

Strategy to pick reference points by placing them on the axis ends.

This strategy produces $n+2$ reference points that lie on the edges of the surrounding cube.
**Full Database Reference Points**
de.lmu.ifi.dbs.elki.utilities.referencepoints.FullDatabaseReferencePoints
Strategy to use the complete database as reference points.

**Grid Based Reference Points**
de.lmu.ifi.dbs.elki.utilities.referencepoints.GridBasedReferencePoints
Grid-based strategy to pick reference points.

**Random Generated Reference Points**
de.lmu.ifi.dbs.elki.utilities.referencepoints.RandomGeneratedReferencePoints
Reference points generated randomly within the used data space.

**Random Sample Reference Points**
de.lmu.ifi.dbs.elki.utilities.referencepoints.RandomSampleReferencePoints
Random-Sampling strategy for picking reference points.

**Star Based Reference Points**
de.lmu.ifi.dbs.elki.utilities.referencepoints.StarBasedReferencePoints
Star-based strategy to pick reference points.

### J.5 Scaling

de.lmu.ifi.dbs.elki.utilities.scaling package:
Scaling functions: linear, logarithmic, gamma, clipping, ...

**Clip Scaling**
de.lmu.ifi.dbs.elki.utilities.scaling.ClipScaling
Scale implementing a simple clipping. Values less than the specified minimum will be set to the minimum, values larger than the maximum will be set to the maximum.

**Gamma Scaling**
de.lmu.ifi.dbs.elki.utilities.scaling.GammaScaling
Non-linear scaling function using a Gamma curve.

**Identity Scaling**
de.lmu.ifi.dbs.elki.utilities.scaling.IdentityScaling
The trivial "identity" scaling function.

**Linear Scaling**
de.lmu.ifi.dbs.elki.utilities.scaling.LinearScaling
Simple linear scaling function.

**Minus Log Scaling**
de.lmu.ifi.dbs.elki.utilities.scaling.MinusLogScaling
Scaling function to invert values by computing \(-1 * \text{Math.log(x)}\)

### J.5.1 Outlier

de.lmu.ifi.dbs.elki.utilities.scaling.outlier package:
Scaling of Outlier scores, that require a statistical analysis of the occurring values
COP Outlier Scaling [KKSZ12, KKSZ11] (since 0.6.0)
delmu.ifi.dbs.elki.utilities.scaling.outlier.COPOutlierScaling
CDF based outlier score scaling.
Enhanced version of the scaling proposed in:
Hans-Peter Kriegel, Peer Kröger, Erich Schubert, Arthur Zimek
Interpreting and Unifying Outlier Scores
Proc. 11th SIAM International Conference on Data Mining (SDM 2011)
See also:
Hans-Peter Kriegel, Peer Kröger, Erich Schubert, Arthur Zimek
Outlier Detection in Arbitrarily Oriented Subspaces
in: Proc. IEEE Int. Conf. on Data Mining (ICDM 2012)

HeDES Normalization Outlier Scaling [NAG10] (since 0.4.0)
delmu.ifi.dbs.elki.utilities.scaling.outlier.HeDESNormalizationOutlierScaling
Normalization used by HeDES

Log Ranking Pseudo Outlier Scaling (since 0.7.0)
delmu.ifi.dbs.elki.utilities.scaling.outlier.LogRankingPseudoOutlierScaling
This is a pseudo outlier scoring obtained by only considering the ranks of the objects. However, the ranks are not mapped linearly to scores, but using a normal distribution.

Minus Log Gamma Scaling [KKSZ11] (since 0.3)
delmu.ifi.dbs.elki.utilities.scaling.outlier.MinusLogGammaScaling
Scaling that can map arbitrary values to a probability in the range of [0:1], by assuming a Gamma distribution on the data and evaluating the Gamma CDF.

Minus Log Standard Deviation Scaling [KKSZ11] (since 0.3)
delmu.ifi.dbs.elki.utilities.scaling.outlier.MinusLogStandardDeviationScaling
Scaling that can map arbitrary values to a probability in the range of [0:1]. Transformation is done using the formula \( \max\{0, \text{erf}(\lambda - \mu) / \sqrt{2}\} \)
Where mean can be fixed to a given value, and stddev is then computed against this mean.

Mixture Model Outlier Scaling [GT06] (since 0.4.0)
delmu.ifi.dbs.elki.utilities.scaling.outlier.MixtureModelOutlierScaling
Tries to fit a mixture model (exponential for inliers and gaussian for outliers) to the outlier score distribution. Note: we found this method to often fail, and fit the normal distribution to the inliers instead of the outliers, yielding reversed results.

Multiplicative Inverse Scaling [KKSZ11] (since 0.3)
delmu.ifi.dbs.elki.utilities.scaling.outlier.MultiplicativeInverseScaling
Scaling function to invert values by computing 1/x, but in a variation that maps the values to the [0:1] interval and avoiding division by 0.
The exact formula can be written as
\[
1/(v \cdot \max \frac{1}{|x|}) = \min(|x|)/v
\]
with \(1/0 := 1\)

Outlier Gamma Scaling [KKSZ11] (since 0.3)
delmu.ifi.dbs.elki.utilities.scaling.outlier.OutlierGammaScaling
Scaling that can map arbitrary values to a probability in the range of [0:1] by assuming a Gamma distribution on the values.
Outlier Linear Scaling

Scaling that can map arbitrary values to a value in the range of [0:1]. Transformation is done by linear mapping onto 0:1 using the minimum and maximum values.

Outlier Minus Log Scaling

Scaling function to invert values by computing -log(x) and linear mapping onto 0:1.

Outlier Sqrt Scaling

Scaling that can map arbitrary positive values to a value in the range of [0:1]. Transformation is done by taking the square root, then doing a linear mapping onto 0:1 using the minimum values seen.

Ranking Pseudo Outlier Scaling

This is a pseudo outlier scoring obtained by only considering the ranks of the objects. However, the ranks are not mapped linearly to scores, but using a normal distribution.

Sigmoid Outlier Scaling

Tries to fit a sigmoid to the outlier scores and use it to convert the values to probability estimates in the range of 0.0 to 1.0.

Sqrt Standard Deviation Scaling

Scaling that can map arbitrary values to a probability in the range of [0:1]. Transformation is done using the formulas

\[
y = \sqrt{x - \min} \\
s = \max\{0, \text{erf}\left(\frac{y - \mu}{\sigma \sqrt{2}}\right)\}
\]

Where \(\min\) and mean \(\mu\) can be fixed to a given value, and stddev \(\sigma\) is then computed against this mean.

Standard Deviation Scaling

Scaling that can map arbitrary values to a probability in the range of [0:1]. Transformation is done using the formula

\[
\max\{0, \text{erf}\left(\frac{x - \mu}{\sigma \sqrt{2}}\right)\}
\]

Where mean can be fixed to a given value, and stddev is then computed against this mean.

TopK Outlier Scaling

Outlier scaling function that only keeps the top \(k\) outliers.

K Visualization

Visualization package of ELKI.
K.1 Parallel3d

`de.lmu.ifi.dbs.elki.visualization.parallel3d` package:
3DPC: 3D parallel coordinate plot visualization for ELKI.
This is an add-on module. Details were published as:

**OpenGL3D Parallel Coordinates** [AKSZ13] (since 0.6.0)
`de.lmu.ifi.dbs.elki.visualization.parallel3d.OpenGL3DParallelCoordinates`
Simple JOGL2 based parallel coordinates visualization.

**Parallel 3D Renderer** [AKSZ13] (since 0.6.0)
`de.lmu.ifi.dbs.elki.visualization.parallel3d.Parallel3DRenderer`
Renderer for 3D parallel plots.
The tricky part here is the vertex buffer layout. We are drawing lines, so we need two vertices for each macro edge (edge between axes in the plot). We furthermore need the following properties: we need to draw edges sorted by depth to allow alpha and smoothing to work, and we need to be able to have different colors for clusters. An efficient batch therefore will consist of one edge-color combination. The input data comes in color-object ordering, so we need to seek through the edges when writing the buffer. In total, we have $2 \cdot \text{obj.size} \cdot \text{edges.size}$ vertices.
Where $\text{obj.size} = \text{sum}(\text{col.sizes})$

K.1.1 Layout

`de.lmu.ifi.dbs.elki.visualization.parallel3d.layout` package:
Layouting algorithms for 3D parallel coordinate plots.

**Compact Circular MST Layout 3DPC** [AKSZ13] (since 0.6.0)
`de.lmu.ifi.dbs.elki.visualization.parallel3d.layout.CompactCircularMSTLayout3DPC`
Simple circular layout based on the minimum spanning tree.

**Multidimensional Scaling MST Layout 3DPC** [AKSZ13] (since 0.6.0)
`de.lmu.ifi.dbs.elki.visualization.parallel3d.layout.MultidimensionalScalingMSTLayout3DPC`
Layout the axes by multi-dimensional scaling.

**Simple Circular MST Layout 3DPC** [AKSZ13] (since 0.6.0)
`de.lmu.ifi.dbs.elki.visualization.parallel3d.layout.SimpleCircularMSTLayout3DPC`
Simple circular layout based on the minimum spanning tree.

K.2 Projector

`de.lmu.ifi.dbs.elki.visualization.projector` package:
Projectors are responsible for finding appropriate projections for data relations.

**Histogram Factory** (since 0.4.0)
`de.lmu.ifi.dbs.elki.visualization.projector.HistogramFactory`
Produce one-dimensional projections.

**OPTICS Projector Factory** (since 0.4.0)
`de.lmu.ifi.dbs.elki.visualization.projector.OPTICSProjectorFactory`
Produce OPTICS plot projections
Parallel Plot Factory

delmu.ifidi.fbs.elski.visualization.projector.ParallelPlotFactory

Produce parallel axes projections.

Parallel Plot Projector

delmu.ifidi.fbs.elski.visualization.projector.ParallelPlotProjector

ParallelPlotProjector is responsible for producing a parallel axes visualization.

Scatter Plot Factory

delmu.ifidi.fbs.elski.visualization.projector.ScatterPlotFactory

Produce scatterplot projections.

K.3 Visualizers

delmu.ifidi.fbs.elski.visualization.visualizers package:

Visualizers for various results

K.3.1 Actions

delmu.ifidi.fbs.elski.visualization.visualizers.actions package:

Action-only ‘visualizers’ that only produce menu entries.

Cluster Style Action

delmu.ifidi.fbs.elski.visualization.visualizers.actions.ClusterStyleAction

Actions to use clusterings for styling.

K.3.2 Histogram

delmu.ifidi.fbs.elski.visualization.visualizers.histogram package:

Visualizers based on 1D projected histograms.

Colored Histogram Visualizer

delmu.ifidi.fbs.elski.visualization.visualizers.histogram.ColoredHistogramVisualizer

Generates a SVG-Element containing a histogram representing the distribution of the database’s objects.

K.3.3 Optics

delmu.ifidi.fbs.elski.visualization.visualizers.optics package:

Visualizers that do work on OPTICS plots

OPTICS Cluster Visualization

delmu.ifidi.fbs.elski.visualization.visualizers.optics.OPTICSClusterVisualization

Visualize the clusters and cluster hierarchy found by OPTICS on the OPTICS Plot.

OPTICS Plot Cut Visualization

delmu.ifidi.fbs.elski.visualization.visualizers.optics.OPTICSPlotCutVisualization

Visualizes a cut in an OPTICS Plot to select an Epsilon value and generate a new clustering result.

OPTICS Plot Selection Visualization

delmu.ifidi.fbs.elski.visualization.visualizers.optics.OPTICSPlotSelectionVisualization

Handle the marker in an OPTICS plot.
OPTICS Plot Visualizer (since 0.3)
de.lmu.ifi.dbs.elki.visualization.visualizersOPTICSPlotVisualizer
Visualize an OPTICS result by constructing an OPTICS plot for it.

OPTICS Steep Area Visualization (since 0.4.0)
de.lmu.ifi.dbs.elki.visualization.visualizersOPTICSSteepAreaVisualization
Visualize the steep areas found in an OPTICS plot

K.3.4 Pairsegments

de.lmu.ifi.dbs.elki.visualization.visualizerspairsegments package:
Visualizers for inspecting cluster differences using pair counting segments.

Circle Segments Visualizer (AGK+12) (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizerspairsegmentsCircleSegmentsVisualizer
Visualizer to draw circle segments of clusterings and enable interactive selection of segments. For "empty" segments, all related segments are selected instead, to visualize the differences.

K.3.5 Parallel

de.lmu.ifi.dbs.elki.visualization.visualizersparallel package:
Visualizers based on parallel coordinates.

Axis Reorder Visualization (since 0.5.5)
de.lmu.ifi.dbs.elki.visualization.visualizersparallelAxisReorderVisualization
Interactive SVG-Elements for reordering the axes.

Axis Visibility Visualization (since 0.5.5)
de.lmu.ifi.dbs.elki.visualization.visualizersparallelAxisVisibilityVisualization
Layer for controlling axis visibility in parallel coordinates.

Bounding Box Visualization (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizersparallelBoundingBoxVisualization
Draw spatial objects (except vectors!)

Line Visualization (since 0.7.0)
de.lmu.ifi.dbs.elki.visualization.visualizersparallelLineVisualization
Generates data lines.

Parallel Axis Visualization (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizersparallelParallelAxisVisualization
Generates a SVG-Element containing axes, including labeling.

Parallel Cluster de.lmu.ifi.dbs.elki.visualization.visualizersparallel.cluster package:
Visualizers for clustering results based on parallel coordinates.

Cluster Outline Visualization (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizersparallel.clusterClusterOutlineVisualization
Generates a SVG-Element that visualizes the area covered by a cluster.
Cluster Parallel Mean Visualization  
\[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.parallel.cluster.} \text{ClusterParallelMeanVisualization}\]  
Generates a SVG-Element that visualizes cluster means.

Parallel Index  \[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.parallel.index}\]  
Visualizers for index structure based on parallel coordinates.

R Tree Parallel Visualization  \[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.parallel.index.RTreeParallelVisualization}\]  
Visualize the of an R-Tree based index.

Parallel Selection  \[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.parallel.selection}\]  
Visualizers for object selection based on parallel projections.

Selection Axis Range Visualization  \[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.parallel.selection.SelectionAxisRangeVisualization}\]  
Visualizer for generating an SVG-Element representing the selected range.

Selection Line Visualization  \[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.parallel.selection.SelectionLineVisualization}\]  
Visualizer for generating SVG-Elements representing the selected objects.

Selection Tool Axis Range Visualization  \[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.parallel.selection.SelectionToolAxisRangeVisualization}\]  
Tool-Visualization for the tool to select axis ranges.

Selection Tool Line Visualization  \[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.parallel.selection.SelectionToolLineVisualization}\]  
Tool-Visualization for the tool to select objects.

K.3.6 Scatterplot  
\[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot}\]  
Visualizers based on scatterplots.

Axis Visualization  \[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.AxisVisualization}\]  
Generates a SVG-Element containing axes, including labeling.

Marker Visualization  \[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.MarkerVisualization}\]  
Visualize e.g. a clustering using different markers for different clusters. This visualizer is not constraint to clusters. It can in fact visualize any kind of result we have a style source for.

Polygon Visualization  \[\text{de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.PolygonVisualization}\]  
Renders PolygonsObject in the data set.
Reference Points Visualization (since 0.4.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.ReferencePointsVisualization
The actual visualization instance, for a single projection

Tooltip Score Visualization (since 0.4.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.TooltipScoreVisualization
Generates a SVG-Element containing Tooltips. Tooltips remain invisible until their corresponding Marker is touched by the cursor and stay visible as long as the cursor lingers on the marker.

Tooltip String Visualization (since 0.4.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.TooltipStringVisualization
Generates a SVG-Element containing Tooltips. Tooltips remain invisible until their corresponding Marker is touched by the cursor and stay visible as long as the cursor lingers on the marker.

Scatterplot Cluster
dejmu.ifi.dbs.elki.visualization.visualizers.scatterplot.cluster
class:
Visualizers for clustering results based on 2D projections.

Cluster Hull Visualization (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.cluster.ClusterHullVisualization
Visualizer for generating an SVG-Element containing the convex hull / alpha shape of each cluster.

Cluster Mean Visualization (since 0.7.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.cluster.ClusterMeanVisualization
Visualize the mean of a KMeans-Clustering

Cluster Order Visualization (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.cluster.ClusterOrderVisualization
Cluster order visualizer: connect objects via the spanning tree the cluster order represents.

Cluster Star Visualization (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.cluster.ClusterStarVisualization
Visualize the mean of a KMeans-Clustering using stars.

EM Cluster Visualization (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.cluster.EMClusterVisualization
Visualizer for generating SVG-Elements containing ellipses for first, second and third standard deviation. In more than 2-dimensional data, the class tries to approximate the cluster extends.

Voronoi Visualization (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.cluster.VoronoiVisualization
Visualizer drawing Voronoi cells for k-means clusterings.
See also: KMeans clustering

Scatterplot Density
dejmu.ifi.dbs.elki.visualization.visualizers.scatterplot.density
package:
Visualizers for data set density in a scatterplot projection.
Density Estimation Overlay
[Sc092] (since 0.3)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.density.DensityEstimationOverlay
A simple density estimation visualization, based on a simple kernel-density in the projection, not the actual data!

Scatterplot Index
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.index package:
Visualizers for index structures based on 2D projections.

Tree MBR Visualization (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.index.TreeMBRVisualization
Visualize the bounding rectangles of an R-Tree based index.

Tree Sphere Visualization (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.index.TreeSphereVisualization
Visualize the bounding sphere of a metric index.

Scatterplot Outlier
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.outlier package:
Visualizers for outlier scores based on 2D projections.

Bubble Visualization
[AKR+10] (since 0.5.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.outlier.BubbleVisualization
Generates a SVG-Element containing bubbles. A Bubble is a circle visualizing an outlierness-score, with its center at the position of the visualized object and its radius depending on the objects score.

COP: Correlation Outlier Probability
[KKSZ12] (since 0.5.5)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.outlier.COPVectorVisualization
Visualize error vectors as produced by COP.

Scatterplot Selection
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.selection package:
Visualizers for object selection based on 2D projections.

Distance Function Visualization (since 0.5.5)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.selection.DistanceFunctionVisualization
Factory for visualizers to generate an SVG-Element containing dots as markers representing the kNN of the selected Database objects.
To use this, add a kNN preprocessor index to your database!

Move Objects Tool Visualization (since 0.4.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.selection.MoveObjectsToolVisualization
Tool to move the currently selected objects.

Selection Convex Hull Visualization (since 0.4.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.selection.SelectionConvexHullVisualization
Visualizer for generating an SVG-Element containing the convex hull of the selected points
Selection Cube Visualization  
(de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.selection.SelectionCube) 
Visualizer for generating an SVG-Element containing a cube as marker representing the selected range for each dimension.

Selection Dot Visualization  
(de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.selection.SelectionDot) 
Visualizer for generating an SVG-Element containing dots as markers representing the selected Database’s objects.

Selection Tool Cube Visualization  
(de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.selection.SelectionToolCube) 
Tool-Visualization for the tool to select ranges.

Selection Tool Dot Visualization  
(de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.selection.SelectionToolDot) 
Tool-Visualization for the tool to select objects.

Scatterplot Uncertain  
(de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.uncertain) 
Visualizers for uncertain data.

Uncertain Bounding Box Visualization  
(de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.uncertain.UncertainBoundingBox) 
Visualize uncertain objects by their bounding box.
Note: this is currently a hack. Our projection only applies to vector field relations currently, and this visualizer activates if such a relation (e.g. a sample, or the center of mass) has a parent relation of type UncertainObject. But it serves the purpose.

Uncertain Instances Visualization  
(de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.uncertain.UncertainInstances) 
Visualize a single derived sample from an uncertain database.
Note: this is currently a hack. Our projection only applies to vector field relations currently, and this visualizer activates if such a relation (e.g. a sample, or the center of mass) has a parent relation of type UncertainObject. But it serves the purpose.

Uncertain Samples Visualization  
(de.lmu.ifi.dbs.elki.visualization.visualizers.scatterplot.uncertain.UncertainSamples) 
Visualize uncertain objects by multiple samples.
Note: this is currently a hack. Our projection only applies to vector field relations currently, and this visualizer activates if such a relation (e.g. a sample, or the center of mass) has a parent relation of type UncertainObject. But it serves the purpose.

K.3.7  Visunproj 
(de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj) 
Visualizers that do not use a particular projection.
Dendrogram Visualization (since 0.7.5)
de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj.DendrogramVisualization
Dendrogram visualizer.

Evaluation Visualization (since 0.4.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj.EvaluationVisualization
Pseudo-Visualizer, that lists the cluster evaluation results found.

Histogram Visualization (since 0.3)
de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj.HistogramVisualization
Visualizer to draw histograms.

Key Visualization (since 0.3)
de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj.KeyVisualization
Visualizer, displaying the key for a clustering.

Label Visualization (since 0.3)
de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj.LabelVisualization
Trivial "visualizer" that displays a static label. The visualizer is meant to be used for dimension labels in the overview.

Pixmap Visualizer (since 0.4.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj.PixmapVisualizer
Visualize an arbitrary pixmap result.

Settings Visualization (since 0.3)
de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj.SettingsVisualization
Pseudo-Visualizer, that lists the settings of the algorithm-

Similarity Matrix Visualizer (since 0.4.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj.SimilarityMatrixVisualizer
Visualize a similarity matrix with object labels

XY Curve Visualization (since 0.3)
de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj.XYCurveVisualization
Visualizer to render a simple 2D curve such as a ROC curve.

XY Plot Visualization (since 0.7.0)
de.lmu.ifi.dbs.elki.visualization.visualizers.visunproj.XYPlotVisualization
Visualizer to render a simple 2D curve such as a ROC curve.
References

[ABD+08] Elke Achtert, Christian Böhm, Jörn David, Peer Kröger, and Arthur Zimek. Robust clustering in arbitrarily oriented subspaces. In SDM, pages 763–774, 2008.

[ABK+06a] Elke Achtert, Christian Böhm, Hans-Peter Kriegel, Peer Kröger, Ina Müller-Gorman, and Arthur Zimek. Finding hierarchies of subspace clusters. In PKDD, pages 446–453, 2006.

[ABK+06b] Elke Achtert, Christian Böhm, Hans-Peter Kriegel, Peer Kröger, and Arthur Zimek. Deriving quantitative models for correlation clusters. In KDD, pages 4–13, 2006.

[ABK06c] Elke Achtert, Christian Böhm, and Peer Kröger. Deli-clu: Boosting robustness, completeness, usability, and efficiency of hierarchical clustering by a closest pair ranking. In PAKDD, pages 119–128, 2006.

[ABK+07a] Elke Achtert, Christian Böhm, Hans-Peter Kriegel, Peer Kröger, Ina Müller-Gorman, and Arthur Zimek. Detection and visualization of subspace cluster hierarchies. In DASFAA, pages 152–163, 2007.

[ABK+07b] Elke Achtert, Christian Böhm, Hans-Peter Kriegel, Peer Kröger, and Arthur Zimek. On exploring complex relationships of correlation clusters. In SSDBM, page 7, 2007.

[ABK+07c] Elke Achtert, Christian Böhm, Hans-Peter Kriegel, Peer Kröger, and Arthur Zimek. Robust, complete, and efficient correlation clustering. In SDM, pages 413–418, 2007.

[ABKS99] Mihael Ankerst, Markus M. Breunig, Hans-Peter Kriegel, and Jörg Sander. Optics: Ordering points to identify the clustering structure. In SIGMOD Conference, pages 49–60, 1999.

[ABKZ06] Elke Achtert, Christian Böhm, Peer Kröger, and Arthur Zimek. Mining hierarchies of correlation clusters. In SSDBM, pages 119–128, 2006.

[ACF+15] Laurent Amsaleg, Oussama Chelly, Teddy Furon, Stéphane Girard, Michael E. Houle, Ken-ichi Kawasaki, and Michael Nett. Estimating local intrinsic dimensionality. In KDD, pages 29–38, 2015.

[Ach01] Dimitris Achlioptas. Database-friendly random projections. In PODS, 2001.

[AD52] T. W. Anderson and D. A. Darling. Asymptotic theory of certain "goodness of fit" criteria based on stochastic processes. The Annals of Mathematical Statistics, 23(2):193–212, 1952.

[AD74] Joachim H. Ahrens and Ulrich Dieter. Computer methods for sampling from gamma, beta, poisson and bionomial distributions. Computing, 12(3):223–246, 1974.

[AD82] Joachim H. Ahrens and Ulrich Dieter. Generating gamma variates by a modified rejection technique. Commun. ACM, 25(1):47–54, 1982.

[AGAV09] Enrique Amigó, Julio Gonzalo, Javier Artilés, and Felisa Verdejo. A comparison of extrinsic clustering evaluation metrics based on formal constraints. Inf. Retr., 12(5):613, 2009.

[AGGR98] Rakesh Agrawal, Johannes Gehrke, Dimitrios Gunopulos, and Prabhakar Raghavan. Automatic subspace clustering of high dimensional data for data mining applications. In SIGMOD Conference, pages 94–105, 1998.

[AGK+12] Elke Achtert, Sascha Goldhofer, Hans-Peter Kriegel, Erich Schubert, and Arthur Zimek. Evaluation of clusterings - metrics and visual support. In IEEE 28th International Conference on Data Engineering (ICDE 2012), Washington, DC, USA (Arlington, Virginia), 1-5 April, 2012, pages 1285–1288, 2012.

[AIS93] Rakesh Agrawal, Tomasz Imielski, and Arun N. Swami. Mining association rules between sets of items in large databases. In SIGMOD Conference, pages 207–216, 1993.

[Aka73] Hirotogu Akaike. Information theory and an extension of the maximum likelihood principle. In Proceedings of the 2nd International Symposium on Information Theory, pages 267–281, 1973.
Elke Achtert, Hans-Peter Kriegel, Lisa Reichert, Erich Schubert, Remigius Wojdanowski, and Arthur Zimek. Visual evaluation of outlier detection models. In *Database Systems for Advanced Applications, 15th International Conference, DASFAA 2010, Tsukuba, Japan, April 1-4, 2010, Proceedings, Part II*, pages 396–399, 2010.

Elke Achtert, Hans-Peter Kriegel, Erich Schubert, and Arthur Zimek. Interactive data mining with 3d-parallel-coordinate-trees. In *Proceedings of the ACM SIGMOD International Conference on Management of Data, SIGMOD 2013, New York, NY, USA, June 22-27, 2013*, pages 1009–1012, 2013.

Michael R. Anderberg. *Cluster Analysis for Applications*, chapter Hierarchical Clustering Methods. 1973.

Michael R. Anderberg. *Cluster Analysis for Applications*, chapter Nonhierarchical Clustering Methods. 1973.

Fabrizio Angiulli and Clara Pizzuti. Fast outlier detection in high dimensional spaces. In *PKDD*, pages 15–26, 2002.

Rakesh Agrawal and Ramakrishnan Srikant. Fast algorithms for mining association rules in large databases. In *VLDB*, pages 487–499, 1994.

Chuan-Heng Ang and T. C. Tan. New linear node splitting algorithm for r-trees. In *SSD*, pages 339–349, 1997.

David Arthur and Sergei Vassilvitskii. k-means++: the advantages of careful seeding. In *SODA*, pages 1027–1035, 2007.

Charu C. Aggarwal, Joel L. Wolf, Philip S. Yu, Cecilia Procopiuc, and Jong Soo Park. Fast algorithms for projected clustering. *ACM SIGMOD Record*, 28(2):61–72, 1999.

Charu C. Aggarwal and Philip S. Yu. Finding generalized projected clusters in high dimensional spaces. In *SIGMOD Conference*, pages 70–81, 2000.

Charu C. Aggarwal and Philip S. Yu. Outlier detection for high dimensional data. In *SIGMOD Conference*, pages 37–46, 2001.

Sio Iong Ao, Kevin Y. Yip, Michael K. Ng, David Wai-Lok Cheung, Pui-Yee Fong, Ian Melhado, and Pak Chung Sham. Clustag: hierarchical clustering and graph methods for selecting tag snps. *Bioinformatics*, 21(8):1735–1736, 2005.

Amit Bagga and Breck Baldwin. Entity-based cross-document coreferencing using the vector space model. In *Proceedings of the 17th international conference on Computational linguistics*, 1998.

J. Roger Bray and J. T. Curtis. An ordination of the upland forest communities of southern wisconsin. *Ecological Monographs*, 27(4):325–349, 1957.

Donald J. Berndt and James Clifford. Using dynamic time warping to find patterns in time series. In *KDD Workshop*, pages 359–370, 1994.

J. Beirlant, G. Dierckx, and A. Guillou. Estimation of the extreme-value index and generalized quantile plots. *Bernoulli*, 11(6):949–970, 2005.

Jon Louis Bentley. Multidimensional binary search trees used for associative searching. *Commun. ACM*, 18(9):509–517, 1975.

J. M. Bernardo. Algorithm as 103: Psi (digamma) function. *Applied Statistics*, 25(3):315, 1976.

Paul S. Bradley and Usama M. Fayyad. Refining initial points for k-means clustering. In *ICML*, pages 91–99, 1998.

Leo Breiman, Jerome H. Friedman, R. A. Olshen, and Charles J. Stone. *Classification and Regression Trees*. Wadsworth, 1984.
Frank B. Baker and Lawrence J. Hubert. Measuring the power of hierarchical cluster analysis. *Journal of the American Statistical Association*, 70(349):31–38, 1975.

Stefan Berchtold, Daniel A. Keim, and Hans-Peter Kriegel. The $\chi$-tree: An index structure for high-dimensional data. In *VLDB*, pages 28–39, 1996.

Christian Böhm, Karin Kailing, Hans-Peter Kriegel, and Peer Kröger. Density connected clustering with local subspace preferences. In *ICDM*, pages 27–34, 2004.

Christian Böhm, Karin Kailing, Peer Kröger, and Arthur Zimek. Computing clusters of correlation connected objects. In *SIGMOD Conference*, pages 455–466, 2004.

Alina Beygelzimer, Sham Kakade, and John Langford. Cover trees for nearest neighbor. In *ICML*, pages 97–104, 2006.

Markus M. Breunig, Hans-Peter Kriegel, Raymond T. Ng, and Jörg Sander. Optics-of: Identifying local outliers. In *PKDD*, pages 262–270, 1999.

Markus M. Breunig, Hans-Peter Kriegel, Raymond T. Ng, and Jörg Sander. LoF: Identifying density-based local outliers. In *SIGMOD Conference*, pages 93–104, 2000.

Thomas Bernecker, Hans-Peter Kriegel, Matthias Renz, Florian Verhein, and Andreas Züle. Probabilistic frequent itemset mining in uncertain databases. In *KDD*, pages 119–128, 2009.

Norbert Beckmann, Hans-Peter Kriegel, Ralf Schneider, and Bernhard Seeger. The $r^*$-tree: An efficient and robust access method for points and rectangles. In *SIGMOD Conference*, pages 322–331, 1990.

Paul S. Bradley, Olvi L. Mangasarian, and W. Nick Street. Clustering via concave minimization. In *NIPS*, pages 368–374, 1996.

Sergey Brin, Rajeev Motwani, and Craig Silverstein. Beyond market baskets: Generalizing association rules to correlations. In *SIGMOD Conference*, pages 265–276, 1997.

Sergey Brin, Rajeev Motwani, Jeffrey D. Ullman, and Shalom Tsur. Dynamic itemset counting and implication rules for market basket data. In *SIGMOD Conference*, pages 255–264, 1997.

M. Basseville and I. V. Nikiforov. *Detection of Abrupt Changes - Theory and Application*, chapter Section 2.6: Off-line Change Detection. 1993.

Christian Baumgartner, Claudia Plant, Karin Kailing, Hans-Peter Kriegel, and Peer Kröger. Subspace selection for clustering high-dimensional data. In *ICDM*, pages 11–18, 2004.

D. J. Best and D. E. Roberts. Algorithm as 91: The percentage points of the $\chi^2$ distribution. *Applied Statistics*, 24(3):385, 1975.

Leo Breiman. Bagging predictors. *Machine Learning*, 24(2):123–140, 1996.

Omar Benjelloun, Anish Das Sarma, Alon Y. Halevy, and Jennifer Widom. Uldbs: Databases with uncertainty and lineage. In *VLDB*, pages 953–964, 2006.

Jacob Bien and Robert Tibshirani. Hierarchical clustering with prototypes via minimax linkage. *Journal of the American Statistical Association*, 106(495):1075–1084, 2011.

D. Blackman and S. Vigna. xoroshiro+ / xorshift* / xorshift+ generators and the prng shootout, 2016.

Ergun Biçici and Deniz Yuret. Locally scaled density based clustering. In *ICANNGA (1)*, pages 739–748, 2007.

D. Bilková. Lognormal distribution and using I-moment method for estimating its parameters. *Int. Journal of Mathematical Models and Methods in Applied Sciences (NAUN)*, 1(6), 2012.

George Casella and Roger L. Berger. *Statistical Inference*, chapter Point Estimation. Duxbury, 1990.
[CC00] Yizong Cheng and George M. Church. Biclustering of expression data. In ISMB, pages 93–103, 2000.

[CCKN06] Michael Chau, Reynold Cheng, Ben Kao, and Jackey Ng. Uncertain data mining: An example in clustering location data. In PAKDD, pages 199–204, 2006.

[CCVR16] Richard C. H. Connor, Franco Alberto Cardillo, Lucia Vadicamo, and Fausto Rabitti. Hilbert exclusion: Improved metric search through finite isometric embeddings. CoRR, abs/1604.08640, 2016.

[CG13] Sanjay Chawla and Aristides Gionis. k-means-: A unified approach to clustering and outlier detection. In SDM, pages 189–197, 2013.

[CH74] T. Calinski and J. Harabasz. A dendrite method for cluster analysis. Communications in Statistics - Theory and Methods, 3(1):1–27, 1974.

[Cha02] Moses Charikar. Similarity estimation techniques from rounding algorithms. In STOC, pages 380–388, 2002.

[Che95] Yizong Cheng. Mean shift, mode seeking, and clustering. IEEE Trans. Pattern Anal. Mach. Intell., 17(8):790–799, 1995.

[CHK16] Oussama Chelly, Michael E. Houle, and Ken-ichi Kawarabayashi. Enhanced estimation of local intrinsic dimensionality using auxiliary distances. Technical report, National Institute of Informatics, 2016.

[CLB10] Feng Chen, Chang-Tien Lu, and Arnold P. Boedihardjo. Gls-sod: a generalized local statistical approach for spatial outlier detection. In KDD, pages 1069–1078, 2010.

[CMS13] Ricardo J. G. B. Campello, Davoud Moulavi, and Jörg Sander. Density-based clustering based on hierarchical density estimates. In PAKDD (2), pages 160–172, 2013.

[CN04] Lei Chen and Raymond T. Ng. On the marriage of lp-norms and edit distance. In VLDB, pages 792–803, 2004.

[COO05] Lei Chen, M. Tamer Özsu, and Vincent Oria. Robust and fast similarity search for moving object trajectories. In SIGMOD Conference, pages 491–502, 2005.

[Cor71] R. M. Cormack. A review of classification. Journal of the Royal Statistical Society. Series A (General), 134(3):321, 1971.

[CPZ97] Paolo Ciaccia, Marco Patella, and Pavel Zezula. M-tree: An efficient access method for similarity search in metric spaces. In VLDB, pages 426–435, 1997.

[CS06] Sanjay Chawla and Pei Sun. Slom: a new measure for local spatial outliers. Knowl. Inf. Syst., 9(4):412–429, 2006.

[CW69] S. C. Choi and R. Wette. Maximum likelihood estimation of the parameters of the gamma distribution and their bias. Technometrics, 11(4):683, 1969.

[Dar57] D. A. Darling. The kolmogorov-smirnov, cramer-von mises tests. The Annals of Mathematical Statistics, 28(4):823–838, 1957.

[DB79] David L. Davies and Donald W. Bouldin. A cluster separation measure. IEEE Trans. Pattern Anal. Mach. Intell., 1(2):224–227, 1979.

[DCL11] Wei Dong, Moses Charikar, and Kai Li. Efficient k-nearest neighbor graph construction for generic similarity measures. In WWW, pages 577–586, 2011.

[DD09] Elena Deza and Michel Marie Deza. Encyclopedia of Distances. Springer Berlin Heidelberg, 2009.

[Def77] D. Defays. An efficient algorithm for a complete link method. Comput. J., 20(4):364–366, 1977.

[Dic45] Lee R. Dice. Measures of the amount of ecologic association between species. Ecology, 26(3):297–302, 1945.
[DIIM04] Mayur Datar, Nicole Immorlica, Piotr Indyk, and Vahab S. Mirrokni. Locality-sensitive hashing scheme based on p-stable distributions. In Symposium on Computational Geometry, pages 253–262, 2004.

[DLPT85] E. Diday, J. Lemaire, J. Pouget, and F. Testu. Elements d’analyse de donnees. Dunod, 1985.

[DLR77] A. P. Dempster, N. M. Laird, and D. B. Rubin. Maximum likelihood from incomplete data via the EM algorithm. Journal of the Royal Statistical Society, Series B, 39(1), 1977.

[Dra13] Jonathan Drake. Faster k-means clustering. Master’s thesis, Baylor University, 2013.

[DRS09] Nilesh N. Dalvi, Christopher Ré, and Dan Suciu. Probabilistic databases: diamonds in the dirt. Commun. ACM, 52(7):86–94, 2009.

[dRTD98] D. de Ridder, D. M. J. Tax, and R. P. W. Duin. An experimental comparison of one-class classification methods. In Proc. 4th Ann. Conf. Advanced School for Computing and Imaging (ASCI’98), 1998.

[dVCH10] Timothy de Vries, Sanjay Chawla, and Michael E. Houle. Finding local anomalies in very high dimensional space. In ICDM, pages 128–137, 2010.

[EKSX96] Martin Ester, Hans-Peter Kriegel, Jörg Sander, and Xiaowei Xu. A density-based algorithm for discovering clusters in large spatial databases with noise. In KDD, pages 226–231, 1996.

[Elk03] Charles Elkan. Using the triangle inequality to accelerate k-means. In ICML, pages 147–153, 2003.

[ES03] Dominik Maria Endres and Johannes E. Schindelin. A new metric for probability distributions. IEEE Trans. Information Theory, 49(7):1858–1860, 2003.

[Esk00] Eleazar Eskin. Anomaly detection over noisy data using learned probability distributions. In ICML, pages 255–262, 2000.

[ESK03] Levent Eröz, Michael Steinbach, and Vipin Kumar. Finding clusters of different sizes, shapes, and densities in noisy, high dimensional data. In SDM, pages 47–58, 2003.

[FB81] Martin A. Fischler and Robert C. Bolles. Random sample consensus: A paradigm for model fitting with applications to image analysis and automated cartography. Commun. ACM, 24(6):381–395, 1981.

[FD07] B. J. Frey and D. Dueck. Clustering by passing messages between data points. Science, 315(5814):972–976, 2007.

[Fis36] R. A. Fisher. The use of multiple measurements in taxonomic problems. Annals of Eugenics, 7(2):179–188, 1936.

[FLP+51] K. Florek, J. Łukaszewicz, J. Perkal, H. Steinhaus, and S. Zubrzycki. Sur la liaison et la division des points d’un ensemble fini. Colloquium Mathematicae, 2(3-4):282–285, 1951.

[FM83] E. B. Fowlkes and C. L. Mallows. A method for comparing two hierarchical clusterings. Journal of the American Statistical Association, 78(383):553, 1983.

[For65] E. W. Forgy. Cluster analysis of multivariate data: efficiency versus interpretability of classifications. Biometrics, 21(3), 1965.

[FR07] Chris Fraley and Adrian E. Raftery. Bayesian regularization for normal mixture estimation and model-based clustering. J. Classification, 24(2):155–181, 2007.

[GBSM02] Fernando Berzal Galiano, Ignacio J. Blanco, Daniel Sánchez, and María Amparo Vila Miranda. Measuring the accuracy and interest of association rules: A new framework. Intell. Data Anal., 6(3):221–235, 2002.

[Gow67] J. C. Gower. A comparison of some methods of cluster analysis. Biometrics, 23(4):623, 1967.

[Gra72] Ronald L. Graham. An efficient algorithm for determining the convex hull of a finite planar set. Inf. Process. Lett., 1(4):132–133, 1972.
[Gre89] Diane Greene. An implementation and performance analysis of spatial data access methods. In ICDE, pages 606–615, 1989.

[GT06] Jing Gao and Pang-Ning Tan. Converting output scores from outlier detection algorithms into probability estimates. In ICDM, pages 212–221, 2006.

[Guo03] Diansheng Guo. Coordinating computational and visual approaches for interactive feature selection and multivariate clustering. Information Visualization, 2(4):232–246, 2003.

[Gut84] Antonin Guttman. R-trees. ACM SIGMOD Record, 14(2):47, 1984.

[HA85] Lawrence Hubert and Phipps Arabie. Comparing partitions. Journal of Classification, 2(1):193–218, 1985.

[Ham50] R. W. Hamming. Error detecting and error correcting codes. Bell System Technical Journal, 29(2):147–160, 1950.

[Ham74] Frank R. Hampel. The influence curve and its role in robust estimation. Journal of the American Statistical Association, 69(346):383, 1974.

[Ham10] Greg Hamerly. Making k-means even faster. In SDM, pages 130–140, 2010.

[Har75] John A. Hartigan. Clustering Algorithms, chapter Quick Partition Algorithms: Leader Algorithm, page 75. Wiley, 1975.

[HD14] Greg Hamerly and Jonathan Drake. Accelerating Lloyd’s algorithm for k-means clustering. In Partitional Clustering Algorithms, pages 41–78. 2014.

[Hel09] E. Hellinger. Neue begründung der theorie quadratischer formen von unendlichvielen veränderlichen. Journal für die reine und angewandte Mathematik, 1909.

[Hen06] Monika Rauch Henzinger. Finding near-duplicate web pages: a large-scale evaluation of algorithms. In SIGIR, pages 284–291, 2006.

[HH07] Robert M. Haralick and Rave Harpaz. Linear manifold clustering in high dimensional spaces by stochastic search. Pattern Recognition, 40(10):2672–2684, 2007.

[Hil91] D. Hilbert. Ueber die stetige abbildung einer linie auf ein flächenstück. Mathematische Annalen, 38(3):210–271, 1891.

[Hil75] Bruce M. Hill. A simple general approach to inference about the tail of a distribution. The Annals of Statistics, 3(3):1163–1174, 1975.

[HKF04] Ville Hautamäki, Ismo Kärkkäinen, and Pasi Fränti. Outlier detection using k-nearest neighbour graph. In ICPR (3), pages 430–433, 2004.

[HKKP01] Ronald Huisman, Kees G Koedijk, Clemens J. M Kool, and Franz Palm. Tail-index estimates in small samples. Journal of Business & Economic Statistics, 19(2):208–216, 2001.

[HKN12] Michael E. Houle, Hisashi Kashima, and Michael Nett. Generalized expansion dimension. In ICDM Workshops, pages 587–594, 2012.

[HL76] Lawrence J. Hubert and Joel R. Levin. A general statistical framework for assessing categorical clustering in free recall. Psychological Bulletin, 83(6):1072–1080, 1976.

[HMTW47] Cecil Hastings, Frederick Mosteller, John W. Tukey, and Charles P. Winsor. Low moments for small samples: A comparative study of order statistics. The Annals of Mathematical Statistics, 18(3):413–426, 1947.

[Hoe48] W. Hoeffding. A non-parametric test of independence. The Annals of Mathematical Statistics, 19, 1948.

[Hos00] J. R. M. Hosking. Fortran routines for use with the method of l-moments version 3.03. Technical report, IBM, 2000.
[HPY00] Jiawei Han, Jian Pei, and Yiwen Yin. Mining frequent patterns without candidate generation. In *SIGMOD Conference*, pages 1–12, 2000.

[HQ04] Tianqiang Huang and Xiaolin Qin. Detecting outliers in spatial database. In *ICIG*, pages 556–559, 2004.

[HR02] Geoffrey E. Hinton and Sam T. Roweis. Stochastic neighbor embedding. In *NIPS*, pages 833–840, 2002.

[HS54] Brian Hopkins and J. G. Skellam. A new method for determining the type of distribution of plant individuals. *Annals of Botany*, 18(2):213–227, 1954.

[HS95] Gisli R. Hjaltason and Hanan Samet. Ranking in spatial databases. In *SSD*, pages 83–95, 1995.

[HS03] Tianming Hu and Sam Yuan Sung. Detecting pattern-based outliers. *Pattern Recognition Letters*, 24(16):3059–3068, 2003.

[HS04] Tianming Hu and Sam Yuan Sung. A trimmed mean approach to finding spatial outliers. *Intell. Data Anal.*, 8(1):79–95, 2004.

[HSE+95] James L. Hafner, Harpreet S. Sawhney, William Equitz, Myron Flickner, and Wayne Niblack. Efficient color histogram indexing for quadratic form distance functions. *IEEE Trans. Pattern Anal. Mach. Intell.*, 17(7):729–736, 1995.

[HSZ18] Michael E. Houle, Erich Schubert, and Arthur Zimek. On the correlation between local intrinsic dimensionality and outlierness. In *SISAP*, pages 177–191, 2018.

[HW97] J. R. M. Hosking and James R. Wallis. *Regional Frequency Analysis*. Cambridge University Press, 1997.

[HWW85] J. R. M. Hosking, J. R. Wallis, and E. F. Wood. Estimation of the generalized extreme-value distribution by the method of probability-weighted moments. *Technometrics*, 27(3):251–261, 1985.

[HXD03] Zengyou He, Xiaofei Xu, and Shengchun Deng. Discovering cluster-based local outliers. *Pattern Recognition Letters*, 24(9-10):1641–1650, 2003.

[Ins09] Alfred Inselberg. *Parallel Coordinates*. Springer New York, 2009.

[Jac02] Paul Jaccard. Distribution de la florine alpine dans la bassin de dranses et dans quelques regions voisines. *Bulletin del la Société Vaudoise des Sciences Naturelles*, 1902.

[Jan66] R. C. Jancey. Multidimensional group analysis. *Australian Journal of Botany*, 14(1):127, 1966.

[Jef46] H. Jeffreys. An invariant form for the prior probability in estimation problems. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 186(1007):453–461, 1946.

[JHPvdH12] J. Janssens, F. Huszár, E. Postma, and J. van den Herik. Stochastic outlier selection. Technical report, Tilburg University, 2012.

[JK02] Kalervo Järvelin and Jaana Kekäläinen. Cumulated gain-based evaluation of ir techniques. *ACM Trans. Inf. Syst.*, 20(4):422–446, 2002.

[Joh67] Stephen C. Johnson. Hierarchical clustering schemes. *Psychometrika*, 32(3):241–254, 1967.

[JOT+05] H. V. Jagadish, Beng Chin Ooi, Kian-Lee Tan, Cui Yu, and Rui Zhang. idistance: An adaptive b. *ACM Trans. Database Syst.*, 30(2):364–397, 2005.

[JTHW06] Wen Jin, Anthony K. H. Tung, Jiawei Han, and Wei Wang. Ranking outliers using symmetric neighborhood relationship. In *PAKDD*, pages 577–593, 2006.

[JTSF00] Caetano Traina Jr., Agma J. M. Traina, Bernhard Seeger, and Christos Faloutsos. Slim-trees: High performance metric trees minimizing overlap between nodes. In *EDBT*, pages 51–65, 2000.

[KF93] Ibrahim Kamel and Christos Faloutsos. On packing r-trees. In *CIKM*, pages 490–499, 1993.
William Klement, Peter A. Flach, Nathalie Japkowicz, and Stan Matwin. Smooth receiver operating characteristics (smroc) curves. In ECML/PKDD (2), pages 193–208, 2011.

Peer Kröger, Hans-Peter Kriegel, and Karin Kailing. Density-connected subspace clustering for high-dimensional data. In SDM, pages 246–256, 2004.

Hans-Peter Kriegel, Peer Kröger, Matthias Schubert, and Ziyue Zhu. Efficient query processing in arbitrary subspaces using vector approximations. In SSDBM, pages 184–190, 2006.

Hans-Peter Kriegel, Peer Kröger, Erich Schubert, and Arthur Zimek. A general framework for increasing the robustness of pca-based correlation clustering algorithms. In SSDBM, pages 418–435, 2008.

Hans-Peter Kriegel, Peer Kröger, Erich Schubert, and Arthur Zimek. Loop: local outlier probabilities. In CIKM, pages 1649–1652, 2009.

Hans-Peter Kriegel, Peer Kröger, Erich Schubert, and Arthur Zimek. Outlier detection in axis-parallel subspaces of high dimensional data. In PAKDD, pages 831–838, 2009.

Hans-Peter Kriegel, Peer Kröger, Erich Schubert, and Arthur Zimek. Interpreting and unifying outlier scores. In SDM, pages 13–24, 2011.

Hans-Peter Kriegel, Peer Kröger, Erich Schubert, and Arthur Zimek. Outlier detection in arbitrarily oriented subspaces. In ICDM, pages 379–388, 2012.

J. Kuan and P. Lewis. Fast k nearest neighbour search for r-tree family. In Proceedings of ICICS, 1997 International Conference on Information, Communications and Signal Processing, 1997.

Willi Klösgen. Explora: A multipattern and multistrategy discovery assistant. In Advances in Knowledge Discovery and Data Mining, pages 249–271. 1996.

Fabian Keller, Emmanuel Müller, and Klemens Böhm. Hics: High contrast subspaces for density-based outlier ranking. In ICDE, pages 1037–1048, 2012.

Edwin M. Knorr and Raymond T. Ng. Algorithms for mining distance-based outliers in large datasets. In VLDB, pages 392–403, 1998.

Eamonn J. Keogh and Michael J. Pazzani. Derivative dynamic time warping. In SDM, pages 1–11, 2001.

Hans-Peter Kriegel and Martin Pfeifle. Density-based clustering of uncertain data. In KDD, pages 672–677, 2005.

Leonard Kaufman and Peter J. Rousseeuw. Clustering large data sets. In Pattern Recognition in Practice, pages 425–437. 1986.

Leonard Kaufman and Peter J. Rousseeuw. Statistical Data Analysis Based on the L1-Norm and Related Methods, chapter Clustering by means of Medoids, pages 405–416. North-Holland, 1987.

Leonard Kaufman and Peter J. Rousseeuw. Finding Groups in Data, chapter Clustering Large Applications (Program CLARA), pages 126–163. John Wiley & Sons, Inc., 1990.

Leonard Kaufman and Peter J. Rousseeuw. Finding Groups in Data, chapter Agglomerative Nesting (Program AGNES), pages 199–252. John Wiley & Sons, Inc., 1990.

Leonard Kaufman and Peter J. Rousseeuw. Finding Groups in Data, chapter Partitioning Around Medoids (Program PAM), pages 68–125. John Wiley & Sons, Inc., 1990.

Marie Kratz and Sidney I. Resnick. The qq-estimator and heavy tails. Communications in Statistics. Stochastic Models, 12(4):699–724, 1996.

Hans-Peter Kriegel, Matthias Schubert, and Arthur Zimek. Angle-based outlier detection in high-dimensional data. In KDD, pages 444–452, 2008.
[KSZ17] Hans-Peter Kriegel, Erich Schubert, and Arthur Zimek. The (black) art of runtime evaluation: Are we comparing algorithms or implementations? Knowl. Inf. Syst., 52(2):341–378, 2017.

[Kul59] Solomon Kullback. Information Theory and Statistics. Dover, 1959.

[LCK03a] Chang-Tien Lu, Dechang Chen, and Yufeng Kou. Algorithms for spatial outlier detection. In ICDM, pages 597–600, 2003.

[LCK03b] Chang-Tien Lu, Dechang Chen, and Yufeng Kou. Detecting spatial outliers with multiple attributes. In ICTAI, pages 122–128, 2003.

[LEL97] Scott T. Leutenegger, J. M. Edgington, and Mario A. López. Str: A simple and efficient algorithm for r-tree packing. In ICDE, pages 497–506, 1997.

[Lem16] D. Lemire. Fast random shuffling. Daniel Lemire’s blog, 2016.

[Lin66] V. I. Levenshtein. Binary codes capable of correcting deletions, insertions and reversals. Soviet physics doklady, 10, 1966.

[Lin91] Jianhua Lin. Divergence measures based on the shannon entropy. IEEE Trans. Information Theory, 37(1):145–151, 1991.

[LK05] Aleksandar Lazarevic and Vipin Kumar. Feature bagging for outlier detection. In KDD, pages 157–166, 2005.

[LKC07] Sau Dan Lee, Ben Kao, and Reynold Cheng. Reducing uk-means to k-means. In ICDM Workshops, pages 483–488, 2007.

[LLC10] Xutong Liu, Chang-Tien Lu, and Feng Chen. Spatial outlier detection: random walk based approaches. In GIS, pages 370–379, 2010.

[Llo82] Stuart P. Lloyd. Least squares quantization in pcm. IEEE Trans. Information Theory, 28(2):129–136, 1982.

[LLP07] Longin Jan Latecki, Aleksandar Lazarevic, and Dragoljub Pokrajac. Outlier detection with kernel density functions. In MLDM, pages 61–75, 2007.

[Loa00] C. Loader. Fast and accurate computation of binomial probabilities, 2000.

[LW66] G. N. Lance and W. T. Williams. Computer programs for hierarchical polythetic classification ("similarity analyses"). The Computer Journal, 9(1):60–64, 1966.

[LW67] G. N. Lance and W. T. Williams. A general theory of classificatory sorting strategies: 1. hierarchical systems. The Computer Journal, 9(4):373–380, 1967.

[Mac67] J. MacQueen. Some methods for classification and analysis of multivariate observations. In 5th Berkeley Symp. Math. Statist. Prob., 1967.

[Mah36] P. C. Mahalanobis. On the generalized distance in statistics. Proceedings of the National Institute of Sciences of India, 2(1), 1936.

[Mar04] George Marsaglia. Evaluating the normal distribution. Journal of Statistical Software, 11(4), 2004.

[MASS08] Emmanuel Müller, Ira Assent, Uwe Steinhausen, and Thomas Seidl. Outrank: ranking outliers in high dimensional data. In ICDE Workshops, pages 600–603, 2008.

[McR71] D. J. McRae. Mikca: A fortran iv iterative k-means cluster analysis program. Behavioral Science, 16(4), 1971.

[Mei02] Marina Meilă. Comparing clusterings. Technical Report 418, University of Washington, Seattle, 2002.

[Mei03] Marina Meilă. Comparing clusterings by the variation of information. In COLT, pages 173–187, 2003.
[ORSS06] Rafail Ostrovsky, Yuval Rabani, Leonard Schulman, and Chaitanya Swamy. The effectiveness of Lloyd-type methods for the k-means problem. In 2006 47th Annual IEEE Symposium on Foundations of Computer Science (FOCS’06), 2006.

[ORSS12] Rafail Ostrovsky, Yuval Rabani, Leonard J. Schulman, and Chaitanya Swamy. The effectiveness of lloyd-type methods for the k-means problem. J. ACM, 59(6):28:1–28:22, 2012.

[Pag57] E. S. Page. On problems in which a change in a parameter occurs at an unknown point. Biometrika, 44(1/2):248, 1957.

[PBM04] Malay Kumar Pakhira, Sanghamitra Bandyopadhyay, and Ujjwal Maulik. Validity index for crisp and fuzzy clusters. Pattern Recognition, 37(3):487–501, 2004.

[Pea90] G. Peano. Sur une courbe, qui remplit toute une aire plane. Mathematische Annalen, 36(1), 1890.

[Pet76] A. N. Pettitt. A two-sample anderson-darling rank statistic. Biometrika, 63(1):161–168, 1976.

[Phi02] Steven J. Phillips. Acceleration of anderson-darling rank statistic. Biometrika, 63(1):161–168, 1976.

[Pic85] Dominique Picard. Testing and estimating change-points in time series. Advances in Applied Probability, 17(04):841–867, 1985.

[PJ09] Hae-Sang Park and Chi-Hyuck Jun. A simple and fast algorithm for k-medoids clustering. Expert Syst. Appl., 36(2):3336–3341, 2009.

[PJAM02] Cecilia Magdalena Procopiuc, Michael Jones, Pankaj K. Agarwal, and T. M. Murali. A Monte Carlo algorithm for fast projective clustering. In SIGMOD Conference, pages 418–427, 2002.

[PKGF03] Spiros Papadimitriou, Hiroyuki Kitagawa, Phillip B. Gibbons, and Christos Faloutsos. Loci: Fast outlier detection using the local correlation integral. In ICDE, pages 315–326, 2003.

[PL02] Patrick Pantel and Dekang Lin. Document clustering with committees. In SIGIR, pages 199–206, 2002.

[PM00] Dan Pelleg and Andrew W. Moore. X-means: Extending k-means with efficient estimation of the number of clusters. In ICML, pages 727–734, 2000.

[Pod89] János Podani. New combinatorial clustering methods. In Numerical syntaxonomy, pages 61–77. 1989.

[PPA + 12] Md. Mostofa Ali Patwary, Diana Palsetia, Ankit Agrawal, Wei keng Liao, Fredrik Manne, and Alok N. Choudhary. A new scalable parallel DBSCAN algorithm using the disjoint-set data structure. In SC, page 62, 2012.

[ Pri57] R. C. Prim. Shortest connection networks and some generalizations. Bell System Technical Journal, 36(6):1389–1401, 1957.

[PRTB99] Jan Puzicha, Yossi Rubner, Carlo Tomasi, and Joachim M. Buhmann. Empirical evaluation of dissimilarity measures for color and texture. In ICCV, pages 1165–1172, 1999.

[PS91] Gregory Piatetsky-Shapiro. Discovery, analysis, and presentation of strong rules. In Knowledge Discovery in Databases, pages 229–248. AAAI/MIT Press, 1991.

[PZG06] Yaling Pei, Osman R. Zaïane, and Yong Gao. An efficient reference-based approach to outlier detection in large datasets. In ICDM, pages 478–487, 2006.

[Pé08] P. Pébay. Formulas for robust, one-pass parallel computation of covariances and arbitrary-order statistical moments. Technical Report SAND2008-6212, Sandia National Laboratories, 2008.

[Ran71] William M. Rand. Objective criteria for the evaluation of clustering methods. Journal of the American Statistical Association, 66(336):846, 1971.
[TCFC02] Jian Tang, Zhixiang Chen, Ada Wai-Chee Fu, and David Wai-Lok Cheung. Enhancing effectiveness of outlier detections for low density patterns. In PAKDD, pages 535–548, 2002.

[Ter07] T. B. Teriberry. Computing higher-order moments online, 2007.

[TK00] Pang-Ning Tan and Vipin Kumar. Interestingness measures for association patterns: A perspective. Technical Report 00-036, University of Minnesota, 2000.

[TKS04] Pang-Ning Tan, Vipin Kumar, and Jaideep Srivastava. Selecting the right objective measure for association analysis. Inf. Syst., 29(4):293–313, 2004.

[Top00] Flemming Topsøe. Some inequalities for information divergence and related measures of discrimination. IEEE Trans. Information Theory, 46(4):1602–1609, 2000.

[Vas69] L.N. Vaserstein. Markov processes over denumerable products of spaces describing large systems of automata. Problemy Peredachi Informatsii / Problems of Information Transmission, 5(3), 1969.

[vBHZ15] Jonathan von Brünken, Michael E. Houle, and Arthur Zimek. Intrinsic dimensional outlier detection in high-dimensional data. Technical report, National Institute of Informatics, 2015.

[vdM14] Laurens van der Maaten. Accelerating t-SNE using tree-based algorithms. Journal of Machine Learning Research, 15(1):3221–3245, 2014.

[vdMH08] Laurens J. P. van der Maaten and Geoffrey E. Hinton. Visualizing high-dimensional data using t-SNE. Journal of Machine Learning Research, 9:2579–2605, 2008.

[VHGK03] Michail Vlachos, Marios Hadjieleftheriou, Dimitrios Gunopulos, and Eamonn J. Keogh. Indexing multi-dimensional time-series with support for multiple distance measures. In KDD, pages 216–225, 2003.

[Vig14] S. Vigna. An experimental exploration of marsaglia’s xorshift generators, scrambled, 2014.

[Vin75] T. Vincenty. Direct and inverse solutions of geodesics on the ellipsoid with application of nested equations. Survey Review, 23(176):88–93, 1975.

[vR79] C. J. van Rijsbergen. Information Retrieval. Butterworth, 1979.

[War63] Joe H. Ward. Hierarchical grouping to optimize an objective function. Journal of the American Statistical Association, 58(301):236–244, 1963.

[WB97] R. Weber and S. Blott. An approximation based data structure for similarity search. Technical Report TR1997b, ETH Zentrum, Zürich, 1997.

[Wel62] B. P. Welford. Note on a method for calculating corrected sums of squares and products. Technometrics, 4(3):419, 1962.

[Wes79] D. H. D. West. Updating mean and variance estimates: An improved method. Commun. ACM, 22(9):532–535, 1979.

[WH00] X. Wang and F.J. Hickernell. Randomized halton sequences. Mathematical and Computer Modelling, 32(7-8):887–899, 2000.

[Wil11] E. Williams. Aviation formulary, 2011.

[Wis69] David Wishart. 256. note: An algorithm for hierarchical classifications. Biometrics, 25(1):165, 1969.

[Yar09] V. Yaroslavskiy. Dual-pivot quicksort, 2009.

[YC71] Edward A. Youngs and Elliot M. Cramer. Some results relevant to choice of sum and sum-of-product algorithms. Technometrics, 13(3):657–665, 1971.

[YOTJ01] Cui Yu, Beng Chin Ooi, Kian-Lee Tan, and H. V. Jagadish. Indexing the distance: An efficient method to kNN processing. In VLDB, pages 421–430, 2001.
[YSW09] Bo Yu, Mingqiu Song, and Leilei Wang. Local isolation coefficient-based outlier mining algorithm. In 2009 International Conference on Information Technology and Computer Science, 2009.

[ZCS14] Arthur Zimek, Ricardo J. G. B. Campello, and Jörg Sander. Data perturbation for outlier detection ensembles. In SSDBM, pages 13:1–13:12, 2014.

[ZES+14] Andreas Zülf, Tobias Emrich, Klaus Arthur Schmid, Nikos Mamoulis, Arthur Zimek, and Matthias Renz. Representative clustering of uncertain data. In KDD, pages 243–252, 2014.

[Zha96] T. Zhang. Data clustering for very large datasets plus applications. Technical Report 1355, University of Wisconsin Madison, 1996.

[ZHJ09] Ke Zhang, Marcus Hutter, and Huidong Jin. A new local distance-based outlier detection approach for scattered real-world data. In PAKDD, pages 813–822, 2009.

[Zim08] Arthur Zimek. Correlation Clustering. PhD thesis, Ludwig-Maximilians-Universität München, 2008. Application 2: Outlier Detection (Chapter 18).

[ZJ14] Mohammed J. Zaki and Wagner Meira Jr. Data Mining and Analysis: Fundamental Concepts and Algorithms. Cambridge University Press, 2014.

[ZK01] Y. Zhao and G. Karypis. Criterion functions for document clustering: Experiments and analysis. Technical Report CS 01-040, University of Minnesota, 2001.

[ZPOL97] Mohammed Javeed Zaki, Srinivasan Parthasarathy, Mitsunori Ogihara, and Wei Li. New algorithms for fast discovery of association rules. In KDD, pages 283–286, 1997.

[ZRL96] Tian Zhang, Raghu Ramakrishnan, and Miron Livny. Birch: An efficient data clustering method for very large databases. In SIGMOD Conference, pages 103–114, 1996.

[ZRL97] Tian Zhang, Raghu Ramakrishnan, and Miron Livny. Birch: A new data clustering algorithm and its applications. Data Min. Knowl. Discov., 1(2):141–182, 1997.

[ZXF08] Qinpei Zhao, Mantao Xu, and Pasi Fränti. Knee point detection on bayesian information criterion. In ICTAI (2), pages 431–438, 2008.