Feature Learning for Dimensionality Reduction toward Maximal Extraction of Hidden Patterns

ABSTRACT
Dimensionality reduction (DR) plays a vital role in the visual analysis of high-dimensional data. One main aim of DR is to reveal hidden patterns that lie on intrinsic low-dimensional manifolds. However, DR often overlooks important patterns when the manifolds are distorted or hidden by certain influential data attributes. This paper presents a feature learning framework, FEALM, designed to generate an optimized set of data projections for nonlinear DR in order to capture important patterns in the hidden manifolds. These projections produce maximally different nearest-neighbor graphs so that resultant DR outcomes are significantly different. To achieve such a capability, we design an optimization algorithm as well as introduce a new graph dissimilarity measure, named neighbor-shape dissimilarity. Additionally, we develop interactive visualizations to assist comparison of obtained DR results and interpretation of each DR result. We demonstrate FEALM’s effectiveness through experiments and case studies using synthetic and real-world datasets.

Keywords: Dimensionality reduction, feature learning, network comparison, Nelder-Mead optimization, UMAP, visual analytics.

1 INTRODUCTION
High-dimensional data can contain a rich set of observations measured from phenomena. Dimensionality reduction (DR) constitutes a tool for the understanding of the phenomena by visually revealing patterns in the data and facilitating human interpretation of the patterns [4,10,34], leading to important and fundamental insights. Among others, nonlinear DR, such as t-SNE [40] and UMAP [28], is especially helpful when the patterns are hidden in nonlinear structures (or manifolds) and infeasible to be found from conventional depictions of data (e.g., with scatterplot matrices, heatmaps, and parallel coordinates [26]).

However, nonlinear DR is sensitive to an attribute’s influence on manifolds. While nonlinear DR is commonly applied to all available attributes, it may fail to capture patterns underlying manifolds that are apparent only in a particular subset of attributes that are entangled by the relationships among attributes. Although researchers have investigated the effect of attribute selection on linear DR results [30], there is a lack of studies dealing with nonlinear DR as well as the case where manifolds are entangled.

In this work, we complement nonlinear DR methods to enable them to extract various important but subtle patterns in the manifolds embedded in the attributes or combinations of attributes. We first demonstrate that nonlinear DR suffers from the aforementioned problems even when a trivial change in data, such as the inclusion of one additional attribute, is made. We then present a feature learning framework, FEALM, designed to discover latent features of data, with which nonlinear DR produces significantly different results from the one using all the available attributes as they are. These latent features can be constructed with a linear projection that is equivalent to a combination of data scaling and transformation, which are commonly used for data preprocessing [14]. FEALM’s feature learning is performed through the maximization of the differences between data representations (e.g., nearest neighbor graphs) highly related to nonlinear DR results. Within this framework, we design an exemplifying method for UMAP. We develop an algorithm utilizing the Nelder-Mead optimization method (NMM) [13] to find latent features to produce maximally different nearest-neighbor graphs, which are intermediate products of UMAP, and consequently generate diverse UMAP results. To detect the difference of the graphs, we introduce a new graph dissimilarity measure, called neighbor-shape dissimilarity (or NSD). Using this method, analysts can find multiple relevant UMAP results that are difficult to find through manual preprocessing of data.

We further develop an interactive visual interface to allow analysts to flexibly seek more patterns and gain insights from them. The interface depicts the similarities of DR results generated during the optimization process to notify unexplored embeddings. Also, through brushing and linking, analysts can conveniently compare multiple DR results. To help review each DR result, our interface integrates an existing contrastive-learning-based interpretation method [10], which highlights characteristics of a group of instances through comparison with others.

We demonstrate the effectiveness of FEALM, the exemplifying method, and the visual interface through experiments using synthetic datasets and multiple case studies on real-world datasets. We also conduct a performance evaluation to assess the efficiency of NSD and the optimization algorithm. We provide a demonstration video of the interface, detailed evaluation results, and the source code of FEALM in the supplementary material at https://takanori-fujiwara.github.io/fealm/.

In summary, we consider our primary contributions to be:
• a feature learning framework, FEALM, designed to extract a set of latent features for nonlinear DR, each of which produces a significantly different DR result;
• an exemplifying method for UMAP, where we introduce an NMM-based algorithm as well as a graph dissimilarity measure, NSD;
• a visual interface that assists exploration of DR results and interpretation of each DR result; and
• designed examples that illustrate nonlinear DR’s sensitiveness to trivial disturbance to intrinsic manifolds.

2 RELATED WORK
Our work supplements existing DR methods by learning appropriate features from high-dimensional data. Our feature learning optimizes linear transformations through the exploration of various linear subspaces of the original data. We provide the background and relevant works in DR methods and subspace exploration.

2.1 Dimensionality Reduction Methods
DR is widely used for visual exploration of high-dimensional data [30,34]. Many visualization-purpose DR methods aim to reveal overall data distributions (e.g., variances) or patterns (e.g., clusters) in a low-dimensional space. When only performing a linear projection, $\mathbf{X}$, a DR method is categorized as linear DR. More precisely, it produces an embedding (or representation), $\mathbf{Y}$, from input data, $\mathbf{X}$, with $\mathbf{Y} = \mathbf{X} \mathbf{P}$, where $\mathbf{Y} \in \mathbb{R}^{m \times n}$, $\mathbf{X} \in \mathbb{R}^{m \times m'}$, $\mathbf{P} \in \mathbb{R}^{m \times m'}$, and $n, m, m'$ are the numbers of instances, attributes, and latent features, respectively. For example, principal component analysis (PCA) is a well-known linear DR method. While linear DR only captures the linear structure of $\mathbf{X}$, nonlinear DR can uncover the nonlinear structure $\mathbf{Y}$. For example, t-SNE [40] and UMAP [28] aim to preserve local neighborhoods of each instance, which is often difficult when relying only on a linear projection.
Despite the frequent use of the aforementioned DR methods for visual analytics, they may fail to show important patterns when data contains noises or influential attributes to the overall data distribution. Several DR methods have been developed to address this limitation. For example, discriminant analysis [6, 17], such as linear discriminant analysis (LDA), utilizes class information to reduce noises that are irrelevant to class separation. Contrastive learning [2], such as contrastive PCA, compares two datasets to reveal patterns that are more salient in one dataset when compared to another. Unified linear comparative analysis [12] flexibly incorporates the strengths of both discriminant analysis and contrastive learning. However, all these methods require additional information (e.g., class labels) and focus only on revealing patterns related to a well-defined analysis interest (e.g., classification). Thus, these methods would not be suitable when performing an early-stage exploration without complete knowledge of data and/or expected findings, which is an important task that visual analytics should support.

Other than visualization, some of DR methods can be utilized for feature selection and feature learning [49]. For example, PCA and LDA are frequently used in data preprocessing for subsequent machine learning (ML) methods, such as deep neural networks or even other DR methods (e.g., t-SNE), as reducing dimensions is helpful to avoid high computational costs and the curse of dimensionality. As shown in a comprehensive survey by Zebari et al. [49], a large portion of this type of DR targets classification tasks; FEALM can be seen as an unsupervised linear DR method for feature learning. We design FEALM to pre-process data to produce significantly different nonlinear DR results from one obtained using original data as is. FEALM does not require additional information, such as class labels; thus, it supports an early-stage exploration.

2.2 Exploration of Axis-Parallel Subspaces

There are two major types of subspaces: axis-parallel subspaces and linear subspaces. Axis-parallel subspaces are composed of a subset of original data attributes. Thus, there are 2<sup>n</sup> subspaces we can explore. On the other hand, linear subspaces consist of axes obtained through linear projections of original data. Although linear subspaces embrace axis-parallel subspaces, here we only describe studies on axis-parallel subspaces and the rest in Sect. 2.3.

Scatterplot matrices and parallel coordinates are classic visualizations to explore axis-parallel subspaces [26]. A set of methods have been developed to improve these visualizations’ scalability and usability [55, 67]. In response to the increase in the available number of attributes, more efforts have been devoted to comparing a large set of subspaces. A common approach is finding meaningful subspaces with subspace selection, visualizing each subspace’s dissimilarity, and informing patterns seen in each subspace with DR [19, 70, 43]. While this approach uses DR to understand subspaces, Sun et al. [36] investigated subspace selection’s influences on PCA and multidimensional scaling (MDS) results. More comprehensive descriptions of relevant works can be found in a survey by Liu et al. [25].

Subspace clustering [23, 31] in the ML field shares a closely related concept with our work. Subspace clustering aims to find clusters within axis-parallel subspaces. By limiting the use of data to a subset of attributes, subspace clustering can uncover clusters that are hidden by irrelevant attributes. Note that, in the visualization field, “subspace clustering” is often confusingly used to represent clustering of subspaces; however, in standard ML terminology, subspace clustering performs clustering within axis-parallel subspaces.

Our work seeks subspaces that produce significantly different nonlinear DR results to reveal hidden patterns. The work by Sun et al. [36] and subspace clustering methods [23, 31] are closely related to our work in terms of analyzing the subspace change’s influence on data patterns. However, our work is for the use with nonlinear DR methods and provides optimization and visualization methods to find appropriate linear subspaces, which are not limited to axis-parallel subspaces.

2.3 Exploration of Linear Subspaces

To show high-dimensional data distributions in a selected 2D linear subspace, scatterplots and star coordinates are often used with interactive enhancements [26, 44]. We can see linear DR as a method that selects a view suitable to see some characteristics of data (e.g., variance with PCA [15]). Various interactive adjustment methods for linear DR have been introduced, as summarized in surveys [50, 54].

When dealing with many attributes, manually finding informative subspaces becomes almost infeasible. Thus, researchers have designed (semi)automatic and visual recommendations. For example, Wang et al. [44] utilized LDA to suggest star coordinates that show clear cluster separations. Zhou et al. [50] visualized the similarities of original attributes as well as 1D subspaces to help analysts construct interesting subspaces. Gleicher et al. [15] utilized support-vector machines to suggest simple linear subspaces that satisfy specifications provided by analysts. Grassmannian Atlas [25] provides an overview of projection qualities (e.g., skewness) of all 2D subspaces sampled from the Grassmannian manifold. Lehmann and Theisel [24] developed an optimization method to provide a set of 2D subspaces that are significantly different from each other.

Lehmann and Theisel’s work [24] is the most related work as they also aimed to mine various patterns in different subspaces. While theirs only finds and visualizes 2D subspaces (i.e., equivalent to linear DR onto 2D planes), ours searches multidimensional subspaces and uses them as nonlinear DR inputs to uncover patterns hidden in complex data.

3 Motivating Examples

Using UMAP [28] as a representative nonlinear DR method, we provide concrete cases where nonlinear DR misses important data patterns. The datasets that we created, source code for the data generation, and comprehensive experiment results are made available in the supplementary materials [1]. As shown in Fig. 1-a, we first generated a dataset with three attributes, with which instances are placed around two different spherical surfaces. This dataset has approximately 200 blue (Sphere 1) and 100 orange (Sphere 2) instances. The inner sphere corresponding to Sphere 2 has a radius with 40% length of the outer sphere’s radius. Also, small noises are added for the placement of each instance.

When visualizing this dataset in a 2D space, linear DR can only produce a plane cut of the 3D spheres; consequently, we cannot see a clear distinction between them (see Fig. 1-b). Any linear DR causes a similar issue when data has curved shapes, such as those in the Swiss-Rolls dataset [42]. On the other hand, nonlinear DR methods that aim to preserve each instance’s local neighbors such as t-SNE and UMAP can separate Spheres 1 and 2, as shown in Fig. 1-c.

However, even nonlinear DR easily fails to find important patterns when some attributes affect manifolds that contain the corresponding patterns. This situation can happen even with subtle changes in a dataset. To illustrate this, as shown in Fig. 1-d, we generated a new dataset by adding one attribute that has three classes (Classes A–C) having clearly different values. We shuffled the order of the attributes within axis-parallel subspaces. By limiting the use of data to a subset of attributes, subspace clustering can uncover clusters that are hidden by irrelevant attributes. Note that, in the visualization field, “subspace clustering” is often confusingly used to represent clustering of subspaces; however, in standard ML terminology, subspace clustering performs clustering within axis-parallel subspaces.

Our work seeks subspaces that produce significantly different nonlinear DR results to reveal hidden patterns. The work by Sun et al. [36] and subspace clustering methods [23, 31] are closely related to our work in terms of analyzing the subspace change’s influence on data patterns. However, our work is for the use with nonlinear DR methods and provides optimization and visualization methods to find appropriate linear subspaces, which are not limited to axis-parallel subspaces.
attribute), which leads to a clear separation of Spheres 1–2. Similarly, by assigning a large weight only to the 3-class attribute, DR can find Classes A–C. In fact, our method for UMAP, which we introduce in Sect. 5, can reveal these two patterns by automatically adjusting the weights. Fig. 2 shows three examples suggested by our method. The results are produced with the same UMAP’s hyperparameters as those used in Fig. 1-e. In Fig. 2-c1, by using a relatively small weight for the 3-class attribute (i.e., 0.2), UMAP shows clear clusters of Spheres 1–2. Similarly, Fig. 2-b2 shows three clusters of Classes A–C by assigning the 3-class attribute a large weight.

The above issue can be more complicated when patterns are entangled in multiple attributes’ relationships. We create a dataset exhibiting such a case by adding 20% portions of the 3-class attribute values into one of the 2-sphere attributes and then applying the Z-score normalization again, as described in Fig. 1-g. This type of entanglements can be found in, for example, income statistics partially influenced by age and a political opinion influenced by a voter’s general ideology. The attribute weighting or selection cannot resolve the issue in this dataset. Fig. 3-a1, a2 show UMAP results on this dataset after removing the 3-class attribute, which still do not show the separation of Spheres 1–2. This can be solved by learning latent features by our method. The right two columns of Fig. 3 show a subset of the generated UMAP results. We can see b1 and c2 clearly separate Spheres 1–2 and Classes A–C, respectively.

The above examples demonstrate that nonlinear DR can easily overlook important, obvious data patterns when certain attributes influence intrinsic manifolds—even a single attribute can cause this situation. While the examples are the case for finding distinct data groups, similar issues can happen even when finding, for example, continuous value changes on manifolds as in the Swiss-Rolls dataset.

4 FEALM FRAMEWORK

We introduce a feature learning framework, FEALM, to address the stated issues in nonlinear DR. We name the framework FEALM because it performs FEAture Learning to capture or film patterns underlying hidden Manifolds. As the problem can be overly complicated based on the combinations of DR methods, their hyperparameters, and hidden manifolds we should consider, we first specify our scope. We then describe the architecture of FEALM, where optimized projection matrices are generated with the following steps: (1) constructing a (graph) representation of data, (2) performing optimization to find a projection matrix with which a (graph) representation corresponding to projected data is maximally different from the one constructed in the first step, and (3) repeating the optimized projection matrix generation to produce a maximally different (graph) representation from those obtained so far.

4.1 Problem Scope

FEALM aims to supplement nonlinear DR methods, even more specifically, for those construct a graph-based data representation as their intermediate product or those generate DR results highly related to such a representation. This scope is reasonable and still provides enough flexibility in FEALM because many DR methods can be considered graph-based [28, 46]. Such methods include MDS, the Barnes-Hut t-SNE (common t-SNE implementation) [40], and UMAP [28]. For example, MDS constructs a dissimilarity matrix of instances, which can be converted to a kernel/similarity matrix—corresponding to a weighted graph where nodes and edges represent instances and their similarities, respectively. The Barnes-Hut t-SNE and UMAP perform DR based on a similarity/weighted graph derived from the k-NN graph of instances.

FEALM searches significantly different DR results for a given DR method with given hyperparameters. FEALM is not designed to select a DR method nor hyperparameters to reveal hidden patterns.
FEALM can only find patterns underlying (nonlinear) manifolds that exist in a \textit{linear subspace} of the original data. We set this scope because of two reasons. First, we do not want to allow unintuitive or excessive data manipulation not only to provide more interpretable data preprocessing but also to avoid leading to false patterns as much as possible. A linear projection only allows a set of linear transformations that can be converted into a single matrix multiplication (i.e., $Y = XP$, as described in Sect. 2.1). Based on analysts’ demands, FEALM’s linear projection can be limited to data scaling (or attribute weighting), orthogonal transformation, and a combination of both, all of which are commonly used for data preprocessing. Second, finding hidden manifolds that do not exist in a linear projection of data is computationally challenging. Such manifolds might be able to be found, for example, by utilizing neural networks; however, it requires expensive parameter tuning.

### 4.2 Optimization Architecture

We describe the architecture of FEALM designed with considerations of flexibility and computational efficiency.

#### Forms of the problem.

For input data, $X \in \mathbb{R}^{n \times m}$ ($n$, $m$: the numbers of instances and attributes), latent features can be computed with $XP$, where $P \in \mathbb{R}^{n \times m}$ ($m'$ is the number of latent features and $m' \leq m$) is a projection matrix. With $f_{DR}$, a function that performs DR with a given method and hyperparameters, we can obtain a DR result or representation, $Y_i$, i.e., $Y_i = f_{DR}(XP)$. We can measure a dissimilarity of two DR results, $Y_i$ and $Y_j$, with a certain function, $d_{DR}(Y_i, Y_j)$ (e.g., the Frobenius norm). Let $Y_{0_i}$ denote a DR result using $X$ as is (i.e., $Y_{0_i} = f_{DR}(X)$). Then, we can write an optimization problem to find $P_i$ that generates $Y_1$ maximally different from $Y_{0_i}$ as:

$$\text{argmax}_P d_{DR}(Y_1, Y_{0_i}), \text{ subject to } d_{DR}(Y_i, Y_j) \leq \lambda \text{ for } i \neq j.$$  

(1)

Note that Eq. 1 shares some similarities with the one presented by Lehmann and Theisel [24]. However, their optimization is only to produce 2D linear DR results, and their case limits to $Y_j = XP$ ($P \in \mathbb{R}^{m \times 2}$). Also, they only use the extended version of the Procrustes distance [16] and Frobenius norm as a combination of $d_{DR}$ and $\Phi$ (for more details, refer to [21]). FEALM can be used for nonlinear DR and provides flexibility for each function choice. For $\Phi$, rather than computing a norm or maximum, we recommend taking a minimum of dissimilarities (i.e., $\Phi_{DR}$) maximizes the minimum of dissimilarities). With this, we can find a DR result that is different from all the existing results and avoid a case where the optimization produces the same or similar results (e.g., a case where $Y_{0_i}$ has an extremely larger dissimilarity with $Y_1$ than with other potential DR results). We provide a graphical explanation of such a case in the supplementary materials [1].

While Eq. 1 is a straightforward description of our goal, directly performing this optimization for nonlinear DR methods is often difficult because of two-folded reasons. First, $f_{DR}$ is often computationally expensive. For example, UMAP took 5 seconds to produce Fig. 1h from the data containing only 300 instances and 4 attributes. If the optimization requires many evaluations/trials, completion time can easily surpass several hours (e.g., about 1.5 hours for 1000 evaluations). Second, popularly used nonlinear DR methods such as t-SNE and UMAP contain randomness in $f_{DR}$. For example, random initialization of a representation (as in t-SNE) or random sampling during the optimization (as in UMAP) highly influences the final result [22]. Consequently, it becomes difficult to adjust $P_i$ during the optimization—when the objective value of Eq. 1 becomes better, we do not know whether it is the improvement from changes in $P_i$ or caused by the randomness in $f_{DR}$.

Thus, FEALM also introduces an optimization problem that maximizes the differences among graph representations of data. Here we can use graph representations that are the same with or similar to intermediate products of a given nonlinear DR. This optimization is based on a general observation: if such graph representations have maximal differences, derived DR results are also significantly different. Let $f_{Gr}$ denote a function that generates some graph (e.g., k-NN graph, similarity matrix) from an input matrix. Then, a graph, $G_i$, corresponding to $P_i$ can be obtained with $G_i = f_{Gr}(XP)$. Also, we denote a function that measures a dissimilarity of two graphs, $G_i$ and $G_j$, by $d_{DG}(G_i, G_j)$. With a set of already produced graphs, $G_1, G_2, \ldots, G_e$, we can write a relaxed version of the optimization problem:

$$\text{argmax}_{P_{i+1}} \Phi(d_{DG}(G_{i+1}, G_1), \ldots, d_{DG}(G_{i+1}, G_e)).$$  

(2)

When developing a method within FEALM, we can choose Eq. 1 or Eq. 2 based on the characteristics of a DR method, such as the computational efficiency and stability. We can also use Eq. 1 and 2 in a hybrid manner. For example, we can generate a large amount of projection matrices with Eq. 2 and then filter them with Eq. 1 to obtain refined results.

#### Constraints on a linear projection.

Another important consideration of the optimization is the constraints on $P_i$. We should decide the constraints based on data manipulation allowed for an analysis goal and the optimization difficulty for a given dataset (Sect. 6 provides the detailed discussions). Here we list representative options: (1) no constraint; (2) allowing only data scaling; (3) allowing data scaling and orthogonal transformation. With any option, we can interpret how data is transformed by reviewing values in $P_i$.

When there is (1) no constraint in a projection matrix, $P$, FEALM most flexibly learns features. However, as orthogonality between each learned feature is not guaranteed, distance-related functions (e.g., k-NN graph construction using the Euclidean distance) might be heavily influenced by the distortion. Also, the optimization needs to search the best values for $m \times m'$ parameters in $P$.

When (2) allowing only data scaling, $P = \text{diag}(w)$ where $w$ is an $m$-length vector. Practically, we can restrict $w = \sqrt{m}$ where $u$ is a unit vector. When $u$ consists of uniform values, $w = (1 \cdots 1)^\top$ (i.e., performing no scaling). Then, $w$ can be identified by searching a unit vector. This constraint is used when generating the results in Fig. 2. As this search is only on $m$ parameters, finding the best $P$ is much easier than the case with no constraint. To control how strongly $w$ can be (non)uniform values, we can optionally add a penalty based on the sum of each $P$ column’s L1 norm into Eq. 1 or Eq. 2. More precisely, we set this penalty as $-\lambda_1 |P|_1$, where $\lambda_1 \in \mathbb{R}$, $|P|_1 = (1 \cdots 1) \in \mathbb{R}^m$, and $\lambda_1 = (1 \cdots 1)^\top \in \mathbb{R}^m$. For this constraint, the penalty can also be written as $-\alpha_1 |w|_1$. As $\lambda_1$ becomes a larger positive value, $w$ tends to be more nonuniform values. On the other hand, by using large negative $\lambda_1$, the optimization can produce $w$ with more uniform values (e.g., when $\lambda_1 = -\infty$, $w$ becomes $(1 \cdots 1)^\top$). Using negative $\lambda_1$ is especially effective when we want to avoid generating dissimilar graphs, $G_i$ (or dissimilar DR results, $\lambda$), that can be derived from a selection of few attributes (e.g., when analyzing binary or ordinal data). Note that the L2 norm of $w$ is always constant (i.e., $|w|_2 = \sqrt{m}$ and is not suitable for the regularization.

The last constraint (3) can be written as $P = \text{diag}(w)M\text{diag}(v)$, where $M \in \mathbb{R}^{m \times m}$ is an orthogonal matrix (i.e., $M^\top M = I_m$, $I_m$ is an $m \times m$ identity matrix) and $v$ is an $m'$-length vector. Here $M$ ensures that $\text{diag}(v)$ generates orthogonal features of $X\text{diag}(w)$. And, $v$ weights the features to control their influence on a projection. Similar to $w$, we can decompose $v = \sqrt{v^\top u}$, where $u$ is a unit vector. A projection under this constraint resembles a combination of standard data preprocessing steps (i.e., data scaling and orthogonal data transformation). This constraint still needs to find best $m \times m'$ parameters. Similar to the above data scaling constraint, we can control the sparsity of $P$ with the L1-norm-based penalty. To regulate
the difference of each column in \( P \), we can further add a penalty based on the sum of each \( P \) row’s L2 norm: 
\[-\lambda_2 \frac{1}{m} \sum_{i} \left( (P \circ P) \right)_{i,j} \]  
where \( \lambda_2 \in \mathbb{R} \) and \( \circ \) is the Hadamard product. For example, with large negative \( \lambda_2 \), FEALM generates \( P \) in which each attribute has diverse weights across columns. Note that the sum of each \( P \) row’s L1 norm is equal to the sum of each \( P \) column’s L1 norm; thus, the L2-norm is more suitable to control the differences of the columns. Also, these penalties are optional and can be adjusted based on data’s characteristics (e.g., binary data that easily generates sparse \( P \)).

**General optimization strategies.** Eq. 1 and 2 can be considered as the optimization over manifolds (or often called manifold optimization) \([6, 38]\). For example, for the no constraint option (1), \( P \) can be found from the Euclidean manifold. A solution under the constraint (2) is derived by finding \( u \) from a unit sphere manifold. Lastly, for the constraint (3), we can find \( u, u' \) from unit sphere manifolds and \( M \) from the Grassmann manifold \([38]\) that is a manifold of \( m' \)-dimensional subspaces of \( m \)-dimensional space. To perform manifold optimization, we can utilize existing libraries, such as Pymanopt \([38]\). These libraries can help us, for example, generate parameters on a specified manifold.

To solve the optimization, when all functions involved in Eq. 1 (or Eq. 2) are differentiable, we can use automatic differentiation together with a solver for differentiable functions (e.g., gradient descent) through existing libraries \([38]\). When some functions are not differentiable (e.g., \( k \)-NN graph construction), we can use a derivative-free solver, such as the NMM.

In addition to the problem, constraints, and solver, we need to select or design \( f_{GA}, d_{GR}, \) and/or \( d_{RG} \) based on a DR method.

5 Exemplifying Method

We design an exemplifying method for UMAP, using FEALM. In the rest of the paper, we denote this method **FEALM-UMAP**. We chose UMAP because it is computationally rather efficient (e.g., when compared with t-SNE) \([38]\) and frequently used for visualization in various applications \([7, 11, 22]\). The specific designs for UMAP can also be generalized and easily adapted to other DR methods. For example, we expect that a method for t-SNE can be developed based on FEALM-UMAP with minor adjustments in \( f_{GA} \).

5.1 Graph Generation Function

UMAP processes data in two steps: graph construction and graph layout. Through iterative optimization, the graph layout process performs the placement of instances (often in 2D) based on a constructed graph. This iterative optimization involves random sampling and expensive computations. Thus, we design a method using Eq. 2, which requires \( f_{GA} \) and \( d_{GR} \). During the graph construction process, UMAP computes the instance dissimilarities (by default, using the Euclidean distance) and then produces a \( k \)-NN graph based on the dissimilarities. Afterward, UMAP constructs a fuzzy graph, which is a weighted graph where the dissimilarities are converted to the fuzzy topological representation (refer to \([28]\) for details). From this fact, \( f_{GA} \) can be the generation of a \( k \)-NN or fuzzy graph. While a fuzzy graph contains richer information of instances’ relationships, many of the state-of-the-art graph dissimilarity measures, including those we utilize to design our measure, are only available for unweighted graphs \([27]\). Therefore, we use \( f_{GA} \) that generates a \( k \)-NN graph; however, we can replace this with a fuzzy graph once \( d_{GR} \) suitable for weighted graphs is developed.

5.2 Graph Dissimilarity Measure

We can select a dissimilarity measure for unweighted graphs based on analysis interest. When using nonlinear DR for visualization, however, we usually want to reveal patterns that are visually apparent and related to the instances’ neighborhood relationships (i.e., shape and neighbors), such as clusters and outliers \([30]\). Another critical consideration is computational efficiency as graph comparison itself is often expensive. But, it is difficult to judge only based on theoretical time complexity because of their detailed implementation differences (e.g., requiring only fast matrix operations or slow iterative loops). Based on our experiments \([1]\), we identify that NetLSD \([39]\) can better capture differences of graph shapes with a generally shorter runtime than many other measures available in a library of graph dissimilarities \([27]\). With the eigenvalue-based approximation \([39]\), NetLSD’s time complexity is \( O(qkn + q^2n) \), where \( q \) is the total number of the top and bottom eigenvalues to take for the approximation and \( k \) is the number of neighbors set to generate an \( k \)-NN graph. NetLSD does not consider the neighbor dissimilarity; thus, for \( d_{GR} \), we introduce a new measure, \( NSD \), to capture both neighbor and shape dissimilarities.

5.2.1 Neighbor-Shape Dissimilarity (NSD)

We design a neighbor dissimilarity measure, \( ND \), and combine it with NetLSD to introduce \( NSD \). Fig. 2 and Fig. 4 demonstrate how these measures affect DR results when applying FEALM-UMAP to the same dataset. For example, as seen in Fig. 4-b, ND only considers the changes of \( k \)-neighbors around each instance; as a result, they tend to form similar shapes, where the orders of adjacent nodes are likely different. On the other hand, the results with NetLSD (Fig. 4-a) show different shapes; however, they might not involve many neighborhood changes. Although we need more investigations to precisely conclude these tendencies, due to their algorithms, NetLSD and ND can only address the shape and neighbor differences, respectively. When using NSD (Fig. 2), we can find patterns related to both types of changes.

For the neighbor dissimilarity, one option is to utilize the steadiness and cohesiveness (SnC) \([20]\), which are developed to assess the DR quality by measuring the changes of the neighborhood relationships in the original data and a DR result. While SnC is adaptable to graph comparison, it involves random-walk-based sampling and expensive clustering steps. Thus, similar to the reasons why using Eq. 2 instead of Eq. 1, SnC is not suitable for use in the optimization. Inspired by SnC, we design ND based on shared-nearest neighbor (SNN) similarity \([9]\).

SNN similarity measures how much of neighbors are shared in each pair of instances in a graph. Let \( A \) denote a directed adjacency matrix containing the information of each instance’s \( k \)-NNs. Then, all instance pairs’ SNN similarities, \( S \), can be computed with \( S = AA^\top /k \). Given two graphs, \( G_i \) and \( G_j \), we can obtain the difference of each instance’s SNN similarity with \( D_{ij} \). Let \( D_{ij} \) denote matrices only taking positive and negative values of \( D_{ij} \), respectively. Then, \( D_{ij}^+ \) and \( D_{ij}^- \) capture the increase and decrease of SNNs for each instance in \( G_i \) when compared to \( G_j \). We can compute the total increase and decrease with the Frobenius
norm, i.e., \( \|D_{x_i}\|_p \) and \( \|D_{y_j}\|_p \). Lastly, to reduce them into one value, we take the maximum of them. That is, ND of \( G_i \) and \( G_j \) is defined as:

\[
d_{\text{ND}}(G_i, G_j) = \max(\|D_{x_i}\|_p, \|D_{y_j}\|_p).
\]

Unlike SnC, ND involves only simple matrix computations while keeping a similar strength to SnC to capture the neighbor dissimilarity. We compare SnC and ND in Sect. 6.

Let \( d_{\text{SD}}(d_{\text{SD}} \geq 0) \) denote the shape dissimilarity measure using NetLSd. Since NetLSd is only for undirected graphs, we use undirected k-NN graphs as NetLSd’s inputs (i.e., \( A + A^\top \)), instead of \( A \). Also, by default, we set \( q = 50 \) for the approximation. Then, we define the dissimilarity measured by NSD as:

\[
d_{\text{NSD}}(G_i, G_j) = \min\{\max(\|D_{x_i}\|_p, \|D_{y_j}\|_p) \}
\]

where \( d_{\text{NSD}} \geq 0 \) and \( \beta \) is a hyperparameter that controls how strongly NSD focuses on the neighbor dissimilarity vs. the shape dissimilarity. When \( \beta = 0 \), NSD is equivalent to using NetLSd. As \( \beta \) increases, ND becomes more influential on NSD. Based on our experiment, we set \( \beta = 1 \) by default. \( \beta \) can be adjusted based on the patterns we look for. Since NetLSd involves an exponential function when computing the dissimilarity (refer to (39)), we take a logarithm of \( 1 + d_{\text{SD}} \) (1 is added to avoid taking a logarithm of 0) to avoid excessive influence from the shape difference.

5.3 Optimization

FEALM-UMAP optimizes (Eq. 2) while using the k-NN graph construction as \( \text{f}_\text{GR} \) and \( d_{\text{NSD}} \) as \( \text{d}_\text{GR} \). As recommended, we use \( \text{f}_\text{GR} \) to take a minimum of the dissimilarities. For the constraints of a linear projection, FEALM-UMAP supports all the three representative options described in Sect. 4.2. Since the k-NN graph construction is a non-differentiable function, we develop an NMM-based derivative-free solver. We provide pseudocode in the supplementary material [1].

The optimization by the ordinary NMM begins with initial \( (p+1) \) solutions in a \( p \)-dimensional space, where \( p \) is the number of parameters (i.e., when only allowing data scaling, \( p = m \); for the other cases, \( p = m \times m' \)). The initial solutions are typically generated at random. Then, based on the evaluation of each solution’s objective value, the NMM iteratively moves each solution toward a direction along which a better solution can be likely found while gradually shrinking a searching space. Then, after the user-indicated number of evaluations or the convergence, the NMM returns the best solution so far as a final result. When compared with other derivative-free solvers such as the particle-swarm optimization [21], the NMM does not involve many evaluations of the objective function, and efficiently finds a reasonable solution [48]. By employing the NMM, we can avoid an excessive number of graph dissimilarity calculations.

However, based on the initial solutions, the ordinary NMM easily falls into the local minimum. To mitigate this issue, similar to other hybrid approaches of global and local optimization solvers [48], we incorporate random search optimization into the NMM. Specifically, instead of \( (p+1) \) initial solutions, our solver generates a large number of random solutions (by default, \( 10p+1 \) solutions). Then, the solver selects the \( (p+1) \) best solutions and applies the NMM to them to find the refined solution. For this refining step, to achieve faster convergence than the ordinary NMM for a case with large \( p \) (e.g., \( p > 5 \)), we employ the adaptive NMM introduced by Gao and Han [13]. Even with this adaptive method, the NMM is usually suitable for the optimization involving a considerably small number of parameters (e.g., \( p < 30 \)). Thus, when \( X \) has extremely large \( m \) (e.g., \( m = 100 \)), we recommend preprocessing \( X \) with, for example, PCA or clustering to generate compressed attributes. This type of approaches is often recommended for a complex optimization (e.g., t-SNE [47]) often employs PCA when \( m > 30 \).

Random initialization of solutions and restriction of their movement on a specified manifold (e.g., the Grassmann manifold) can be easily achieved by utilizing the manifold optimization libraries [50].

By repeating the above optimization \( r \) times, we can obtain a set of projection matrices, \( P = \{P_0, \ldots, P_r\} \). When \( r \) is large (e.g., \( r = 100 \)), we can perform spectral clustering [29] on \( P \) to recommend a small number of projections (e.g., 10 projections) that produce significantly different DR results.

5.4 Implementation Details and Complexity Analysis

Implementation. FEALM and FEALM-UMAP are implemented with Python and libraries for matrix computations and optimizations: NumPy/SciPy, Scikit-learn [32], and Pymanopt [38]. While many graph dissimilarities, including NetLSd, are available in netrd [27], we use our implementation, which fully utilizes matrix computations to achieve faster calculation (e.g., our implementation of NetLSd is approximately 20 times faster [1]). Moreover, Pathos is utilized to use multiprocessing for the NMM-based solver.

Time complexity analysis. The k-NN graph construction is used for \( f_{GR} \), which has \( O(n \log(n) m) \) with a ball-tree method [52]. NSD is composed of NetLSd (\( O(kn + q^2 n^2) \)) and ND (\( O(kn^2) \)). Because \( q \leq n \), NSD has \( O(q^2 n + kn^2) \). Thus, when computing the best solution with the NMM, the cost calculation for each solution takes \( O(n(q^2 + kn)) \), where \( r \) is the number of produced graphs so far.

6 Computational Evaluations

We evaluate the performance of computations related to FEALM-UMAP as well as the design of ND by comparing it with SnC [20]. As an experimental platform, we used the MacBook Pro (16-inch, 2019) with 2.3 GHz 8-Core Intel Core i9 (16 threads) and 64 GB 2,667 MHz DDR4. We prepared datasets with the data generation code provided in [12]. From the 20 Newsgroups dataset [8], their code can generate data with various numbers of instances (documents) and attributes (topics) by utilizing the latent Dirichlet allocation. All source code used for the evaluations is available online [1].

Comparison of ND and SnC. We have introduced ND as a faster, more stable alternative to SnC. Here we validate that ND and SnC similarly capture the neighbor changes. Analogous to ND’s \( \|D_{x_i}\|_p \) and \( \|D_{y_j}\|_p \), SnC produces two distinct values, the steadiness and cohesiveness. We define the SnC-based dissimilarity measure as \( d_{\text{SnC}} = 1 - \min(\text{steadiness}, \text{cohesiveness}) \). Note that steadiness and cohesiveness take a range of 0–1; the larger, the fewer changes. For this experiment, we set \( n = 200, m = 10 \), and \( k = 15 \) and randomly generated 500 different projection matrices with the size of \( 10 \times 5 \) and graphs corresponding to the projection matrices (with \( f_{GR}(X) \)).

Fig. 5-a shows \( d_{\text{ND}} \) and \( d_{\text{SnC}} \) of a graph corresponding to the original data and each of the 500 generated graphs. As SnC contains the randomness and \( d_{\text{SnC}} \) can be inconsistent, we took the mean of 50 executions in Fig. 5-a. The mean \( d_{\text{SnC}} \) of 50×50 resulted was 0.20 and the mean of 500 standard deviations was 0.02 (i.e., 10% of the mean). Fig. 5-a presents strong correlations between \( d_{\text{ND}} \) and \( d_{\text{SnC}} \) with Pearson’s and Spearman’s correlation coefficients of 0.73 and 0.72, respectively. Thus, similar to SnC, ND captures the neighbor changes, while ND has no randomness and a significantly smaller computational cost, as discussed in the performance evaluation below. ND’s strengths enable us to provide computationally efficient, stable ND.

Performance of \( f_{GR} \), \( f_{GR} \), \( d_{GR} \), and the optimization. We first evaluate the efficiency of each function related to Eq. 1 and 2 specifically. UMAP (\( f_{GR} \)), k-NN graph construction (\( f_{GR} \), ND (\( d_{GR} \)), NetLSd (\( d_{NSD} \)), NSD (\( d_{NSD} \)), and SnC. The number of instances, \( n \), dominates these functions’ complexities. Thus, we ran the functions with different \( n = 50, 100, \ldots, 3200 \) but fixed \( k, m \), and \( q = 15 \) (UMAP’s default), \( m = 10 \), and \( q = 50 \) (NSD’s default). As we expect many executions for the NMM, we measured the completion time of 1000 executions.

As expected, UMAP and SnC spent much longer completion time than others: e.g., 1616 and 527 seconds, respectively, for 1000
executions when \(n=50\). Therefore, these functions are not suitable to use optimizations that require many evaluations or deal with a larger \(n\)—this is the reason why we have designed Eq. 2 and ND. Other functions’ completion times are shown in Fig. 3-b. We observe that, as \(n\) increases, \(d_{\text{SD}}\) requires more computations, and dominates the completion time of \(d_{\text{ND}}\). However, 1000 executions of \(d_{\text{SD}}\) still can be completed within 520 seconds when \(n=3200\).

We next evaluate the performance of FEALM-UMAP as a whole. In addition to the same settings above, we set \(m^*=2\), no constraint on a projection matrix, and 1000 as the number of objective function evaluations. We then generated a single UMAP result through the optimization (i.e., \(r=1\)). From the result shown in Fig. 5-b, we can see the completion time of FEALM-UMAP generally follows \(d_{\text{SD}}\). Even though FEALM-UMAP involves more computations (e.g., \(k\)-NN graph construction and the solution update for the NMM), FEALM-UMAP is completed faster than \(d_{\text{SD}}\). This is probably because our implementation of the NMM partially employs parallel computations, as described in Sect. 5.4.

**Quality of the optimization.** Similar to the above experiment, we generated a single UMAP result with no constraint. For this experiment, we used the same number of instances (\(n=5000\)) but a different number of attributes \(m=5, 10, 20\). We set \(m^*=2\). Also, to see the effect of the NMM’s settings on the optimization quality, we tested different numbers of evaluations (from 100 to 2000) and initial random solutions \((p+1, 10p+1, 20p+1)\). As we do not know the truly best solution, we analyzed relative accuracy to the optimized solution with large numbers of initial solutions and evaluations, specifically, \((50p+1)\) solutions and 5000 evaluations. We also set a randomly selected solution as the baseline solution. Let \(v\), \(v_{\text{best}}\), and \(v_{\text{base}}\) denote objective values of Eq. 2 for the comparison, best, and baseline solutions, respectively; then, the relative accuracy is \((v-v_{\text{base}})/(v_{\text{best}}-v_{\text{base}})\). As the NMM’s solutions can be varied based on the initialization, we computed each of \(v\), \(v_{\text{best}}\), and \(v_{\text{base}}\) by taking a mean of 10 trials.

Fig. 3-c shows the relative accuracy. Generally, the increase in the number of evaluations improves the accuracies. Also, our hybrid approach using many initial random solutions helps improve the accuracies (e.g., \((10p+1)\) reaches better accuracies than \((p+1)\)). Also, we observe that the relative accuracy tends to be higher for the smaller searching space (e.g., the red lines have higher accuracies). For the \(20\times2\) searching space, the accuracy relative to \(v_{\text{base}}\) is still low even with 2000 executions and \((20p+1)\) initial solutions. Thus, we should use even larger numbers of evaluations and initial solutions to obtain better results. However, as discussed, the NMM is more suitable for a small search space and PCA can be applied for data preprocessing when the original search space is too large. For a small search space, our default parameter, \((10p+1)\) initial solutions, with 1000 evaluations would provide reasonable results.

**7 Visual Interface**

To efficiently investigate FEALM-UMAP’s results, as shown in Fig. 6, we develop a visual user interface (UI), which is also applicable to other methods developed within FEALM. The UI is developed as a web application with Python, JavaScript, and D3. We provide a supplementary demonstration video of the UI [1].

**Exploration of DR results.** The views in Fig. 6-a and b are designed for exploration and comparison of the DR results. Fig. 6-a visualizes the information obtained through the optimization described in Sect. 5.3 including the set of UMAP results (i.e., \(Y\)), dissimilarities of each result (i.e., \(d_{\text{DR}}(Y_{i}, Y_{j})\)), and spectral-clustering-based recommendations. To visually convey the dissimilarities of UMAP results, we generate a 2D plot by applying UMAP based on \(d_{\text{DR}}(Y_{i}, Y_{j})\) (i.e., UMAP on the UMAP results). In this plot, each square point corresponds to a single UMAP result and their spatial proximities represent the similarities of the corresponding UMAP results. We indicate each point’s belonging cluster by coloring each point and the isocontour generated by Bubble Sets [5]. We use black color to distinguish the selected points, which initially correspond to the recommended UMAP results. Also, a point of the original DR (i.e., \(Y_{0}\)) is annotated with the cross mark and text, “OG”. We also support fundamental interactions, such as zooming and tooltoping for previewing UMAP results (e.g., one in Fig. 6-a). A scrollable view in Fig. 6-b shows the UMAP results corresponding to \(Y_{0}\) and the selected black points. Their belonging clusters are indicated with texts and colored boxes (e.g., 7 with the green box). A circle point in each UMAP result represents a data instance. Also, we color these points based on their group labels with a different color scheme from Fig. 6-a. For the comparison, each instance’s color is consistent across all the UMAP results. Analysts can select one UMAP result from this view for more detailed-level investigations, as explained below.

**Interpretation of a DR result.** To help interpret the selected UMAP result, the view in Fig. 6-d shows the information on (1) the projection matrix used to generate the UMAP result and (2) each attribute’s contribution to the characteristics of the group in the UMAP result.

The projection matrix, \(P\), contains the information of more (dis)regarded attributes for the generation of the result. This is useful to understand the cause of the selected UMAP result’s difference from the others. As described in Sect. 4.2, \(P\) can be either diagonal (i.e., \(P = \text{diag}(w)\)) or more dense (i.e., when using no constraint or \(P = \text{diag}(w)M\text{diag}(v)\)). When \(P = \text{diag}(w)\), we visualize values of \(w\) as a bar chart, as shown on the left side of Fig. 6-d. For the other case, we visualize values in \(P\) as a heatmap using a diverging colormap (e.g., Fig. 8-b (left)).

Reviewing patterns shown in the DR result is essential to uncover analytical insights as well as to avoid deriving insights from false patterns due to excessive data transformation. The patterns are often examined through the comparison of data groups in the DR result. To assist group comparison, as shown on the right side of Fig. 6-d, the UI integrates an existing contrastive-learning-based interpretation method, called ccPCA, and the heatmap-based visualization. ccPCA contrasts a target group with a background group to reveal highly-contributed attributes to the characteristics of the target. The attributes’ contributions are obtained as a weight vector, where the larger magnitude, the stronger contribution to the target group’s characteristics. In addition, the sign of the weight vector can represent the direction of the contribution when using the sign adjustment method [11]. For example, while alcohol in Fig. 6-d contributes to the characteristics of both Cultivars 1 and 2, according to their sign, they likely have higher and lower alcohol percentages than others, respectively. Also, to enable the comparison of attribute values of instances, we update the size of each point in Fig. 6-c when a certain attribute name is hovered in Fig. 6-d.

Although the UI uses predefined labels by default (e.g., the cultivar classes in Fig. 6), interactive refinement of groups can be performed with the lasso-selection available in Fig. 6-c and controls shown in Fig. 6-e. The changes in groups automatically update the attributes’ contributions in Fig. 6-d. By default, when computing the contributions with ccPCA, each group is selected as a target group and the other groups are set as one background group. However, the UI also allows the analyst to explicitly select a background group. This functionality is useful when the comparison of two specific groups is more desired.
Through a collective use of the above functionalities and visualizations, we can assess the DR result and patterns. When the observed groups do not result from false patterns, the projection matrix values, attributes' contributions, and distribution of attribute values should show some consistency. This is because the separation visible in the DR result should be highly related to the projection matrix, the differences should be captured in the attributes' contributions, and the attributes' contributions should reflect the attribute value distribution. We provide a concrete example in our case studies.

8 CASE STUDIES
We demonstrate the effectiveness of our approach through case studies on real-world datasets. Throughout all case studies, we generate UMAP results using two different constraints: \( P = \text{diag}(w) \) and \( P = \text{diag}(w)M\text{diag}(v) \). Here we only describe the essential information to present the analysis results. In the supplementary materials [1], we provide all the other details and one additional case study as an analysis example dealing with a large number of attributes (over 700). Note that the patterns uncovered in the case studies are difficult to identify with the aforesaid optimization method by Lehmann and Theisel [24] or attribute selection (refer to [1]).

8.1 Study 1: Diverse Categorization of Wines
We analyze the Wine dataset [8], which consists of 178 instances, 13 attributes, and cultivar labels. As shown in Fig. 6a, DR on this dataset usually reveals three clusters highly related to the cultivars. With FEALM-UMAP, we seek patterns different from those clusters. As shown in Fig. 6b, FEALM-UMAP produces the results with greatly different patterns. We select a UMAP result that contains three clusters (see Fig. 6c). These clusters (especially, the cluster mainly consisting of Cultivar 1) seem to contain different wines from the three clusters in the original UMAP result shown in Fig. 6f. Also, the proximity of each cluster is clearly different from the original UMAP result (e.g., the clusters mainly consisting of Cultivars 1 and 3 are placed close with each other in Fig. 6c). As shown in Fig. 7a1, we interactively define the clusters seen in Fig. 6c as Groups A–C. From the auxiliary information displayed in Fig. 7a2, the UMAP result is generated with the constraint of \( P = \text{diag}(w) \), where ash, ash alkalinity, and magnesium have larger weights than others. Also, these attributes show strong contributions to each clusters’ characteristics, especially for Groups A and C (see Fig. 7).

We further verify the strong associations between the clusters and each of the three attributes. For example, as shown in Fig. 7a1, Group C has small magnesium. According to existing research on this data [3], only these three attributes represent the mineral content of wines. Thus, FEALM-UMAP seems to find a new wine categorization that highly corresponds to the mineral content.

From Fig. 6b, we select a representative UMAP result of DR Cluster 6 (orange) as another categorization example. This result contains multiple clusters, each of which is composed of multiple cultivars. As shown in Fig. 7b1 and b2, we create Groups D–G and visualize the related auxiliary information. From the weights and contributions in Fig. 7b2, we see that multiple attributes, such as malic acid, proanthocyanins, flavanoids, strongly influence the forming of Groups D–G. These attributes are related to wine taste (e.g., proanthocyanins contributes to the dryness) [3]. As low weights are assigned for the attributes related to fermentation (i.e., alcohol and proline), mineral content (e.g., ash), and appearance (e.g., color intensity), we can say that FEALM-UMAP identifies Groups D–G that have the difference more in the taste.
After the above process, 4462 instances are included in who support either the Democratic (see Fig. 8-b (left)), the result is generated with the constraint of transportation/infrastructure are diverse even within each party’s supporters. By assigning large weights to the above attributes while aggregating the influences from certain attributes (e.g., CC20.348a, political ideology), FEALM-UMAP seems to find political subgroups that are difficult to find with the conventional use of DR.

### 9 Discussion

FEALM and FEALM-UMAP have provided a primary step in addressing the stated problem of hidden manifolds. We discuss our approach’s limitations as observed through the theoretical and experimental analyses, and discuss further potential enhancements.

**Scalability and reliability** As discussed in Sect. 5.4 and Sect. 6, FEALM-UMAP has limited scalability for the numbers of instances (n) and attributes (m). Because of NSD’s time complexity, FEALM-UMAP is computationally expensive when m is large. Based on the results in Sect. 6, FEALM-UMAP is practical up until data with a few thousand instances when using a mid-range computer. When m is large, on the other hand, the search space becomes very large; consequently, the NMM requires large numbers of initial solutions and evaluations to find solutions of adequate quality. Thus, we recommend preprocessing with PCA for the case with large m. One potential approach for the efficient optimization is to make all functions differentiable and use derivative-based solvers. We expect that this can be achieved by utilizing differentiable variants of k-neighbor selections as well as developing NSD for weighted graphs. While the equations used in ND and NetLSD can be naturally extended weighted graphs, we need further investigations to understand their characteristics in the context of weighted graphs.

As for the reliability of the generated DR results, similar to other ML methods, FEALM-UMAP could suffer from overfitting when n is relatively small compared to m. Therefore, FEALM-UMAP is suitable for data where n is considerably larger than m (e.g., n = 1000, m = 20). When n is relatively small, we can apply PCA to reduce m or define stronger constraints on the projection matrix (e.g., only data scaling). To further reduce the risk of false findings, our visual interface assists the user to inspect the obtained DR results.

**Generalizability**, FEALM is designed as a general framework for nonlinear DR methods. We emphasize that FEALM is applicable to various nonlinear DR methods, such as t-SNE, as discussed in Sect. 3. FEALM can also be used for linear DR methods. For example, Eq. 1 can be applied to the linear DR method designed by Lehmann and Theisel. Furthermore, we can extend Eq. 2 to recommend sets of graph-related hyperparameters of DR (e.g., the number of neighbors in UMAP), which produce significantly different DR results. This can be achieved by replacing a linear projection matrix with hyperparameters for search parameters.

### 10 Conclusion

We have presented FEALM, a feature learning framework that enables investigation of data patterns via a conjoint use with nonlinear DR. The derived exemplifying method and visual interface have demonstrated the effectiveness of FEALM for analyses of real-world datasets. This work also exposes the limitations of conventional ways of data exploration using dimensionality reduction and thus contributes toward the maximal utilization of data.
