Learning Discriminative Metrics via Generative Models and Kernel Learning

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Abstract

Metrics specifying distances between data points can be learned in a discriminative manner or from generative models. In this paper, we show how to unify generative and discriminative learning of metrics via a kernel learning framework. Specifically, we learn local metrics optimized from parametric generative models. These are then used as base kernels to construct a global kernel that minimizes a discriminative training criterion. We consider both linear and nonlinear combinations of local metric kernels. Our empirical results show that these combinations significantly improve performance on classification tasks. The proposed learning algorithm is also very efficient, achieving order of magnitude speedup in training time compared to previous discriminative baseline methods.

1 Introduction

Metric learning – learning how to specify distances between data points – has been a topic of much interest in machine learning recently. For example, discriminative techniques for metric learning aim to improve the performance of a classifier, such as the k-nearest neighbor classifier, on a training set. As a general strategy, these techniques try to reduce the distances between data points belonging to the same class while increasing the distances between data points from different classes.
a Mahalanobis metric is parameterized by a positive (semi)definite matrix, and metric learning is performed using semi-definite programming (SDP) involving constraints between pairs or triplets of data points in the training set [9].

In the asymptotic limit, the performance of nearest neighbor classifiers approach a theoretical limit, bounded by twice the Bayes optimum error rate, which is independent of the underlying metric used [10]. Only in the finite sampling case does the performance of a nearest neighbor classifier depend upon the choice of a metric, and [11] showed how the bias term can be estimated using simple class-conditional generative models fit to the data. A “generative local metric” (GLM) is then optimized to minimize this bias term.

However, the local metric learning algorithm has several shortcomings. First, a local metric needs to be computed at every point, and it is difficult to calculate the geodesic distance between pairs of distant points. It is also unclear how to correlate the choice of generative models with discriminative classifier performance.

In this paper, we address these issues by combining the learned local metrics in a global discriminative kernel, thus reducing the computational costs for classifying points. Our approach can be viewed as using metric learning to define base kernels which are then combined discriminately [12, 13, 14, 15, 16]. The base kernels are derived from parametric generative models, thus reaping the benefits of both generative and discriminative models [17, 18]. We show how both simple linear and nonlinear combinations result in a highly discriminative global kernel that outperforms competing methods significantly on a number of machine learning datasets. Moreover, we show that our approach is also computationally more efficient than those methods, often achieving orders of magnitude speedup in training time.

The paper is organized as follows. In section 2, we review previous discriminative and generative metric learning techniques. We describe our approach of combining local metrics trained from generative models in section 3. We present extensive empirical studies in section 4, followed by a discussion of our method and future direction in section 5.

The Appendix for this paper includes details of derivations and implementation, more comprehensive empirical results, and applications of our approaches to unsupervised learning problems.

2 Background

Here we briefly review techniques for learning metrics. We start with discriminative metric learning, using the large margin nearest neighbor (LMNN) classifier as an illustrative example [5]. Next, we examine learning a generative local metric (GLM) [11], which exploits information from parametric generative models and does not explicitly attempt to minimize classification errors.

2.1 Discriminative learning metric

Consider a nearest neighbor classifier which labels a D-dimensional data point \( x \in \mathbb{R}^D \) by the label(s) of its nearest neighbor(s) \( x \in D \subset D \) in a supervised training set \( D \). In order to identify the “nearest” neighbors, distances from \( x \) to data points in \( D \) need to be determined.

The conventional Euclidean distance, \( \| x - x' \|^2 \), is a special case of the more general Mahalanobis distance

\[
d_M^2(x, x') = (x - x')^T M (x - x'),
\]

when the Mahalanobis metric \( M \in \mathbb{R}^{D \times D} \) is equal to the D-dimensional identity matrix. In this paper, we follow the popular terminology in the metric learning literature, calling the squared distance as “distance.”

For a general positive semidefinite matrix \( M \), we can factor it as \( M = L^T L \). This implies a general Mahalanobis metric can be interpreted as Euclidean distance in a transformed space, \( x \rightarrow Lx \):

\[
d_M^2(x, x') = (Lx - Lx')^T (Lx - Lx') = \| Lx - Lx' \|^2.
\]

Arguably, the performance of nearest neighbor classifiers depends critically on the metric \( M \). A good \( M \) should intuitively “pull” data points in the same class closer and “push” data points in different classes away. This is the general criteria for most discriminative methods for metric learning [1, 2, 3, 4].
For example, the large margin nearest neighbor (LMNN) classifier casts the learning of \( M \) as a convex optimization problem. For any point \( x_i \) in the training set, it differentiates two sets of neighboring data points: “target” points \( x_i^+ \) whose labels are the same as \( x_i \), and “impostor” points \( x_i^- \) whose labels are different from \( x_i \). LMNN identifies the optimal \( M \) as the solution to,

\[
\min_{M \succeq 0, \xi \geq 0} \sum_i \sum_{j \in x_i^+} d_i^2 M(x_i, x_j) + \gamma \sum_{ijl} \xi_{ijl} \\
\text{subject to} \quad 1 + d_i^2 M(x_i, x_j) - d_i^2 M(x_i, x_l) \leq \xi_{ijl}, \forall j \in x_i^+, l \in x_i^-
\]

where the objective function balances two forces: pulling the targets towards \( x_i \), and pushing the impostors away so that the distance to an impostor should be greater than the distance to the target by a minimum margin of one using the slack variables \( \xi_{ijl} \).

Note that this formulation of LMNN makes no assumptions on how the (training) data is distributed. Additionally, the optimization criterion is directly related to how the learned metric will be used for classification. We see that this approach contrasts sharply with the generative model approach which we describe next.

### 2.2 Generative learning metric

Here we consider a binary classification problem with labels \( y = 1, 2 \), and assume the \( N \) training data points are drawn from two class conditional distributions \( p_1(x) = p(x|y = 1) \) and \( p_2(x) = p(x|y = 2) \). In the asymptotic limit, \( N \to \infty \), the error rate of the nearest neighbor classifier is given in terms of the class conditional distributions.\(^1\)

\[ 
\varepsilon_\infty = \int \frac{p_1(x)p_2(x)}{p_1(x) + p_2(x)} \, dx. \tag{4}
\]

The asymptotic error \( \varepsilon_\infty \) can be easily shown to be invariant to a linear transformation of variables: \( z = Lx \). This implies that learning a different metric \( M \) in Eq. (2) should have no effect on the error rate in the asymptotic limit.

The solution to this apparent paradox is described in [11], which showed that when the number of training points is finite, the error rate of the nearest neighbor classifier deviates from the asymptotic error rate \( \varepsilon_\infty \) by a finite bias term,

\[ 
\varepsilon_N \simeq \varepsilon_\infty + c_N \int \frac{p_1p_2(p_2 - p_1)}{(p_1 + p_2)^2} \left[ \frac{\nabla^2 p_1}{p_1} - \frac{\nabla^2 p_2}{p_2} \right] \, dx \tag{5}
\]

where the constant factor \( c_N \) tends to zero as \( N \) approaches infinity, and the scalar Laplacian \( \nabla^2 p(x) \) is the trace of the Hessian \( \nabla \nabla p(x) \).

This bias term does depend upon the choice of the underlying metric, and under a linear transformation \( z = Lx \), the bias term is given by the integral of

\[ 
\frac{p_1p_2(p_2 - p_1)}{(p_1 + p_2)^2} \text{Trace} \left[ M^{-1} \Phi \right], \quad \text{with} \quad \Phi = \frac{\nabla \nabla p_1(x)}{p_1(x)} - \frac{\nabla \nabla p_2(x)}{p_2(x)}. \tag{6}
\]

The generative local metric (GLM) algorithm optimizes a local metric \( M \) to minimize the local bias term in Eq. (6), so that the finite sample error rate \( \varepsilon_N \) approaches the asymptotic error rate \( \varepsilon_\infty \) to the first-order approximation. The resulting optimization with semidefinite constraints:

\[
\min_{M} \left( \text{Trace} \left[ M_i^{-1} \Phi_i \right] \right)^2, \quad \text{subject to} \quad |M_i| = 1, M_i \succeq 0
\]

is easily solved at each data point \( x_i \) using a spectral decomposition. The optimum \( M_i^* \) is a positive semidefinite matrix whose eigenvectors \( U_i \) are the same as \( \Phi_i \)’s. Then if \( \Lambda^+ \) is the diagonal matrix composed of \( \Phi_i \)’s \( d^+ \) positive eigenvalues, and \( \Lambda^- \) is the corresponding diagonal matrix with \( d^- \) negative eigenvalues.

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\(^1\)For simplicity, we consider equal prior distributions here. Unequal class priors contribute a more complicated scalar term in Eqs. (4)-(6), but the resulting derivation for the optimization of the local metric is unchanged.
eigenvalues, the solution can be written as:

$$M^*_i \propto U_i \left[ \begin{array}{c} d^+ \Lambda^+ \\ -d^- \Lambda^- \end{array} \right] U_i^T$$

where the proportionality constant is determined by scaling the determinant of $M^*_i$ to unity. Note that this learning algorithm does not attempt to reduce the nearest neighbor classification error rate explicitly.

3 Discriminative learning with multiple generative metrics

Prior empirical studies have shown that generative learning metric (GLM) of eq. (8) performs competitively, even when compared to discriminative methods such as the large margin nearest neighbor classifiers (LMNN) [5]. However, GLM has several shortcomings. For every (new) data point $x$ to be classified, the optimization of eq. (8) needs to be solved. The resulting metric $M_x$ depends on $x$ and distances to the training data points need to be computed in this specific metric. While specialized data structures can be exploited to speed up the process of identifying nearest neighbors, these structures usually require a fixed metric and cannot be easily adapted to a new metric [5]. This can significantly increase the computational cost at testing time.

Secondly, the performance of GLM depends on the specific form of the class conditional distributions $p_1(x)$ and $p_2(x)$ used for generative modeling. Initial studies have suggested that even with simplistic models such as Gaussian distributions, GLM attains robust and competitive performance. Nevertheless, rigorously quantifying the relationship between the assumed generative models and the classification performance is lacking. In particular, it is unclear how the choice of the generative models should be adapted in order to further improve the classification performance of the nearest neighbor classifier with the learned metric.

We address these issues by viewing the problem of learning metrics as learning kernels. We then investigate how to improve classification performance by using these kernels. To this end, we consider two schemes for learning kernels discriminatively: linear and nonlinear combination of metrics.

3.1 Linear combination of local metrics

A metric $M_i$ learned at the training point $x_i$ can be seen as a linear positive semidefinite kernel, defining the inner product between two points $x_m$ and $x_n$,

$$K_i(x_m, x_n) = x_m^T M_i x_n$$

Note that while $M_i$ is learned “locally” in the neighborhood of $x_i$, we treat it as an biased estimate of a global kernel function over the space of all training examples. We arrive at an unbiased estimator of the global metric — intuition to be made clear below — by linearly combining all the local metrics learned from the $N$ training samples,

$$K(x_m, x_n) = \sum_i \alpha_i K_i(x_m, x_n) = x_m^T \left( \sum_i \alpha_i M_i \right) x_n = x_m^T M x_n$$

where the combination coefficients $\{ \alpha_i \}_{i=1}^N$ are constrained to be nonnegative and sum to one, guaranteeing the resulting kernel to be positive semidefinite. The global metric $M$ is then simply the convex combination of all local metrics. We now consider the simplest convex combination, uniform averaging:

$$M^{\text{UNI}} = \frac{1}{N} \sum_i M_i$$

As our empirical studies show, this surprisingly simple strategy works well in practice.

As noted earlier, a positive semidefinite metric may be viewed as applying a linear transformation to the original data $x$. This implies that $M^{\text{UNI}}$ transforms $x$ to a new space where on average, local metrics
computed in that space are proportionally to the identity matrix. Thus, on average, the Euclidean distance based nearest neighbor classification will perform well in that space. More formally,

**Theorem 1.** Assume the class conditional distribution \( p_c(x) = p(x|y = c) \) is Gaussian for every class. Let \( M_i \) be the local metric computed with eq. (7), minimizing the bias term in the space of \( x \). Then, the uniform convex combination metric \( M^\text{UNI} \) of eq. (11) induces a linear transformation \( z = Lx \) where \( L^TL = M \). Furthermore, let \( Q_i \) denote the local metric computed in the space of \( z \) under the new class conditional distribution \( p_c(z) \). We have,

\[
\sum_{i=1}^{N} Q_i \propto I
\]

where \( I \) is the identity matrix.

The proof exploits the fact that \( p_c(z) \) is also Gaussian and \( Q_i \) can be expressed as a closed-form expression of \( M_i \). Details are presented in the Appendix (section A).

### 3.2 Nonlinear combination of local metrics

In order to combine local metrics in a nonlinear fashion, we use Gaussian radial basis (RBF) kernel functions to replace the standard identity covariance matrix,

\[
K_{il}(x_m, x_n) = \exp\left\{ -\frac{(x_m - x_n)^T M_i (x_m - x_n)}{\sigma_l^2} \right\}
\]

where \( \sigma_l \) is a bandwidth parameter, chosen from a range of possible values between \( \sigma_{\text{min}} \) and \( \sigma_{\text{max}} \).

Our goal is to learn a convex combination of these RBF base kernels. We follow the standard multiple kernel learning (MKL) framework where base kernels are combined as

\[
K(x_m, x_n) = \sum_{i,l} \alpha_{il} K_{il}(x_m, x_n) \quad \text{subject to } \alpha_{i,l} \geq 0, \sum_{i,l} \alpha_{i,l} = 1
\]

Note that the combined kernel \( K(\cdot, \cdot) \) is a highly nonlinear, albeit convex function of local metrics. It is well-known that positive semidefinite kernels, including ours in eq. (14), can be represented as distances in the corresponding Reproducing Kernel Hilbert Space (RHKS) [19]. However, as opposed to the global metric \( M^\text{UNI} \), we cannot represent this distance (and its associated metric) as a closed-form function of \( x \) and \( \{M_i\}_{i=1}^{N} \).

In typical applications of MKL, one often chooses Gaussian RBF kernels with identity covariance matrices \( \exp(-\|x_m - x_n\|^2/\sigma_l^2) \). This is due to the difficulty in properly choosing non-identity covariance matrices for the base kernels, especially in high-dimensional problems. Our formulation in eq. (14) overcomes the challenge by using non-Euclidean metrics computed from generative modeling.

We refine the combination by optimizing \( \{\alpha_{il}\} \) discriminatively. Specifically, the coefficients \( \{\alpha_{il}\} \) are adjusted so that the kernel \( K(\cdot, \cdot) \) achieves the lowest empirical risk when used in kernel based classifiers such as support vector machines [13]. In this aspect, our formulation reaps the benefits of both generative modeling and discriminative training.

### 3.3 Convex combination: revisited

One may wonder why the framework of multiple kernel learning, used for nonlinear combination of metrics in section 3.2, is not used to discriminatively optimize the convex combination coefficients of eq. (10). Our preliminary results indicate that \( M^\text{UNI} \) in general performs well. This is consistent with previous extensive work on combining kernels linearly — discriminative learning of such combinations does not reliably outperform simpler strategies of combinations including the uniform combination [20, 13]. We present more experimental details, including other forms of convex combinations, in the Appendix (section B). We have found that \( M^\text{UNI} \) is both computationally appealing and empirically very effective.
Table 1: Error rates of misclassification (in %) on the 8 small-scale datasets

| Method | 3-Norm. | Wine | Iris | Heart | Vehi. | Ionos. | Image | German |
|--------|---------|------|------|-------|-------|--------|-------|--------|
| Euclidean | 8.17 | 4.41 | 5.11 | 22.78 | 31.29 | 15.87 | 2.68 | 27.27 |
| LMNN | 4.70 | 2.61 | 4.78 | 21.91 | 21.97 | 12.39 | 2.14 | 27.20 |
| GLM | 3.83 | 3.96 | 3.67 | 21.60 | 25.32 | **6.24** | 2.89 | 26.17 |
| $M^\text{UNI}$ | 3.44 | **1.80** | 3.33 | 19.51 | 17.47 | 9.67 | 2.47 | 26.12 |
| LMNN_E | 3.70 | 2.43 | 4.67 | 20.56 | 20.37 | 11.97 | 2.67 | 26.88 |
| $M^\text{UNI}_E$ | **3.10** | 2.52 | **3.11** | **19.26** | **15.81** | 10.80 | 3.01 | 25.15 |

3.4 Computational complexity and optimization

The computational complexity of our algorithms is dominated by the calculation of local metrics in eq. (8). The main calculation involved is diagonalizing the matrix $\Phi$. For $D$-dimensional space $x$, the computational cost is $O(D^3)$. Since the local metrics are computed at every training sample, the total computational cost is $O(ND^3)$. Computing $M^\text{UNI}$ itself adds little overhead.

In contrast, discriminative techniques such as LMNN for learning a single global metric require iterative numerical optimization. For LMNN, the optimization needs to examine roughly $O(N^3)$ number of constraints. For very large $N$ and small to moderate $D \leq \sqrt{N}$, our approaches will greatly outperform LMNN in speed, as demonstrated later in section 4.

4 Experimental results

We compare our methods of discriminative kernel learning from generative local metrics (GLMs) to other competitive methods of metric learning. Here we report the results of applying simple linear (section 3.1) and nonlinear combinations (section 3.2) to classification. More comprehensive details are included in the Appendix (section B – D).

4.1 Setup

Datasets We have used 10 datasets: 3-Normal, Iris, Wine, Heart, Vehicle, Ionosphere, Image, German, MNIST and Letters. The first 8 datasets are small-scale, having 150–2310 data points with dimensionality ranging from 4 to 34. The number of labelled classes range from 2 to 4. The MNIST and Letters datasets are substantially larger: MNIST has 70,000 deskewed images with 10 classes while Letters has 20,000 examples with 26 labelled classes. 3-Normal is a synthetic set containing a mixture of 3 Gaussians. Other datasets are downloaded from the UCI machine learning repository [21], the IDA benchmark repository[1] and NYU [22].

Data in the small-scale datasets is preprocessed so that the feature vector components range between $-1$ and $1$. For supervised learning tasks such as classification, each dataset is randomly split 30 times into training (60%), validation (20%) and testing (20%) sets.

The MNIST images have a resolution of 784 pixels and are preprocessed with PCA, reducing the dimensionality to 40, 60 and 164 respectively, to save training time and prevent overfitting. We perform 5 random splits, each with 65000 samples for training, 5000 for validation and 10000 for testing. For the Letters dataset, we perform 10 random splits, each with 12000 samples for training, 2000 for validation and 6000 for testing. The Letters-scaled set is with the features scaled to lie within the range $[-1, 1]$. We also provide experimental results on the unscaled version (denoted as Letters-original), as the training time of LMNN is sensitive to the scaling for this dataset.

Learning methods The various learning methods used in our comparative study are summarized be-

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[1]http://www.fml.tuebingen.mpg.de/Members/raetsch/benchmark
• Euclidean. $k$-nearest neighbor ($k$NN) classifier using Euclidean distances.

• LMNN. $k$NN classifier using the metric of Large Margin Nearest Neighbor [5] (cf. section 2).

• GLM$^\text{INT}$. $k$NN classifier using the generative local metrics (GLM) [11] (cf. section 2). Gaussian distributions are used as the class-conditional distributions for generative modeling. We follow the procedure in [11] to interpolate GLM with the Euclidean metric. (Un-interpolated GLMs underperform interpolated ones, a finding which is consistent with what is reported in [11]).

• $M^\text{UNI}$. $k$NN classifier using our approach of uniformly combining the un-interpolated GLMs into a single metric, described by eq. (11).

• LMNN$^E$. Energy-based classification using the metric of LMNN [5].

• $M^\text{UNI}^E$. Energy-based classification using the metric of $M^\text{UNI}$.

Tuning The parameters of all methods are optimized on validation sets, and their overall performance is reported on test sets. Tunable parameters include the number of (target) nearest neighbors, the interpolation parameter in the GLM$^\text{INT}$, and the margins used in the two energy-based classification. We have used the LMNN implementation as reported in [5].

4.2 Linear combination of generative local metrics

Performance on classification tasks Table 1 displays averaged misclassification error rates (over 30 random splits) for the 8 small-scale data sets. Standard errors are reported in the Appendix (section C). The last column is the averaged ranking in performance (across 8 datasets); the smaller the number the better the performance is on average. GLM$^\text{INT}$ outperforms LMNN and Euclidean on most sets, though its performance is surpassed by LMNN$^E$. However, the best performers are $M^\text{UNI}$ and $M^\text{UNI}^E$, which use the simple strategy of uniformly combining the generative local metrics.

Table 2 displays averaged error rates (over 5 random splits for MNIST and 10 for Letters) on large-scale datasets. Standard errors are reported in the Appendix (section C). For the MNIST dataset, we report results on several PCA-preprocessed dimensionality. For Letters, we report results on two cases using scaled and unscaled features.

On the MNIST dataset, it is clear that both $M^\text{UNI}_E$ and LMNN$^E$ perform better than other methods when the dimensionality is low ($D \leq 60$). However, at the larger dimensionality of 164, both LMNN and LMNN$^E$ outperform other methods including our approaches. One possible explanation is that, with the increased dimensionality, the generative modeling used by both GLM$^\text{INT}$ and our approaches ($M^\text{UNI}$ and $M^\text{UNI}^E$), does not fit the data properly. On the other hand, discriminative training might be able to overcome the problem with better regularization.

On the Letters dataset, our approach of $M^\text{UNI}^E$ clearly outperforms all other methods.

Computational efficiency Details are presented in the Appendix (section C.1.1). In summary, we observe that our methods are computationally efficient, achieving orders of magnitude speedup in training time. For example, on MNIST-40, LMNN takes about 40 minutes to learn the final metric while our $M^\text{UNI}$ algorithm takes about 4 minutes.

4.3 Nonlinear combination of generative local metrics

We also report the results of a nonlinear combination of generative local metrics, using the framework of discriminative kernel learning described in section 3.2. The baseline system learns a kernel in the following form $K(x, x') = \sum_l \alpha_l \exp(-\|x - x'\|^2/\sigma_l^2)$ where $\sigma_l$ is the bandwidth of the kernel. Our method of

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2The energy of a point being assigned to a class $c$ is defined as the differences between two quantities: the (sum of) distances of this point to its nearest neighbor in the class $c$ and the (sum of) distances of this point to its nearest neighbor in classes other than $c$. A point is assigned to a class label which has the lowest energy. Energy-based classification can improve performance significantly over $k$NN classification [5].

3 As a comparison point, MNIST-164 has the same dimensionality as the one reported in the work of LMNN [5], with an error rate of 1.37% using the energy-based classification, denoted as LMNN$^E$ in the table. We obtain a similar error rate of 1.34%.
discriminative kernel learning replaces the Euclidean distance in the conventional Gaussian RBF kernel with the generative local metrics (GLMs), as in eq. (13). There are as many local metrics as the number of training examples. Thus, for our implementation, we use “regional” metrics in eq. (13). Specifically, we partition the training data into \( P \) parts. We average local metrics of data points in each part and obtain \( P \) “regional” metrics \( \{ M_p \}_{p=1}^P \). In the specific case where \( P = 1 \), we will get \( M_\text{UNI} \), the uniform linearly combined metric.

For both the baseline method and our approach of kernel learning with eq. (13), the combination coefficients are optimized with the SimpleMKL algorithm [23]. Table 3 displays averaged misclassification error rates on 7 (out of 8) small-scale datasets. Experiments on other datasets are ongoing.

We experiment with different \( P = 1, 5, \) and \( 10 \) and aggregate the results by reporting the best performing \( P \) in Table 3. Further details of our method’s performance with different \( P \) are provided in the Appendix, section C. On 5 out of the 7 datasets, nonlinear combination of metrics clearly outperforms the baseline, with significant improvement on the datasets of 3-Normal, Iris and Vehicle; however, our method performs poorly on the Ionosphere dataset. Note that in Table 1 the local metrics used alone attain a better error rate (6.24%) than the best nonlinear kernel method (6.90%). Thus, more analysis is still needed to understand effective methods for nonlinear combinations of local metrics.

### 4.4 Application to unsupervised learning problems

Many unsupervised learning problems, such as clustering and dimensionality reduction, also rely upon a proper metric to calculate distances. We have also investigated how to apply algorithms to learn metrics to such unsupervised problems. One crucial step is to extract discriminative information from unlabeled data for the algorithms to compute better metrics. To address this issue, we have developed an EM-like procedure to iterate between inferring labels and computing local and global metrics. Details are presented in the Appendix (section D).

We applied this procedure to a number of unsupervised learning problems. We achieve significantly better performance than standard approaches for clustering. Additionally, we can exploit the learned metric for dimensionality reduction, for instance — learning the nonlinear manifold structure of data. As an illustrate example, we show the benefits of using the global metric \( M_\text{UNI} \) with the algorithm of IsoMap [24].

In particular, we compare the IsoMap embedding results computed with the Euclidean metric and the results with the \( M_\text{UNI} \) metric on the MNIST dataset. We selected 400 random samples from different digits ‘3’, ‘5’, and ‘9’, and resized the images to \( 7 \times 7 \). Fig. 1 plots the two different low-dimensional embeddings of data samples, colored according to their digit identities. This clearly shows that learning a global metric helps to discover a better embedding that exhibits clear clustering structure among different class identities.
5 Discussion

In the context of metric learning, we have proposed several new approaches that can reap the benefits of both discriminative training and generative modeling. Our method builds upon the connection between a kernel learning framework and using learned positive semidefinite metrics from generative models as base kernels. Empirical studies validate our algorithms in both improving classification performance across a variety of datasets as well as in computational efficiency in implementation. Ongoing work includes further investigations into more effective approaches to training nonlinear combinations of learned local metrics in a discriminative manner.

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Appendices

A Proof of Theorem 1

Theorem 1: Assume the class conditional distribution \( p_c(x) = p(y|x = c) \) is Gaussian for every class. Let \( M_i \) be the local metric computed with eq. (7), minimizing the bias term in the space of \( x \). Then, the uniformly combined metric \( M^{uni} \) of eq. (17) induces a linear transformation \( z = Lx \) where \( L^T L = M \). Furthermore, let \( Q_i \) denote the local metric computed in the space of \( z \) under the new class conditional distribution \( p_c(z) \). We have,

\[
\sum_{i=1}^{N} Q_i \propto I
\]

where \( I \) is the identity matrix.

Proof. Let \( \Phi_i \) denote the matrix characterizing the bias term on \( x_i \) in the original space (cf. eq. (5)). For multiway classification, the matrix is given by

\[
\Phi = \sum_{c=1}^{C} \nabla \nabla p_i(x) \left( \sum_{c^\prime \neq c} p_{c^\prime i}(x) \sum_{c^\prime \neq c} p_{c^\prime i}(x) \right)
\]

where we have dropped the subscript \( i \) for clarity. For Gaussian class conditional distributions \( p_c(x) = \mathcal{N}(x|\mu_c, \Sigma_c) \), the Hessian \( \nabla \nabla p_c(x) \) is given by

\[
\nabla \nabla p_c(x) = p_c(x) \left[ \Sigma_c^{-1}(x - \mu_c)(x - \mu_c)^T \Sigma_c^{-1} - \Sigma_c^{-1} \right]
\]

Under the linear transformation \( Lx \), the matrix for the bias term in the new space is \( \Psi_i = L^{-1} \Phi_i L^{-T} \). We now establish the relationship between \( Q_i \), which satisfies

\[
\text{Trace } [Q_i^{-1} \Psi_i] = 0, \quad |Q_i| = 1, \quad Q_i \succeq 0
\]

and \( M_i \), the solution in the original space

\[
\text{Trace } [M_i^{-1} \Phi_i] = 0, \quad |M_i| = 1, \quad M_i \succeq 0
\]

Let \( Q_i = |L|^{2/D} L^{-1} M_i L^{-T} \), where \( D \) is the input dimensionality. We claim \( Q_i \) is the solution to eq. (18) as long as \( M_i \) is the solution to eq. (19):

\[
\text{Trace } [Q_i^{-1} \Psi_i] = \text{Trace } [L^T M_i^{-1} LL^{-1} \Phi_i L^{-T}] = \text{Trace } [M_i^{-1} \Phi_i] = 0
\]

and \( |Q_i| = |M_i| = 1, \quad Q_i \succeq 0 \).

Thus, we have,

\[
\sum_i Q_i = |L|^{2/D} \sum_i L^{-1} M_i L^{-T} = N |L|^{2/D} L^{-1} \left( 1/N \sum_i M_i \right) L^{-T}
\]

\[
= N |L|^{2/D} L^{-1} ML^{-T}
\]

Let the eigen-decomposition of \( M \) be \( U \Lambda U^T \), where \( \Lambda = \text{diag}(\lambda_1, ..., \lambda_D) \) contains all eigenvalues and \( U \) contains all eigenvectors. We set \( L = U \Delta U^T \), where \( \Delta = \text{diag}(\sqrt{\lambda_1}, ..., \sqrt{\lambda_D}) \). Then, \( L \) is an induced transformation from \( M \) since \( L^T L = M \). Plugging \( L \) into eq. (22), we obtain:

\[
\sum_i Q_i = N |L|^{2/D} L^{-1} ML^{-T} = N |L|^{2/D} I \propto I
\]
Algorithm 1 Density-based Convex Combination of Local Metrics

1: Compute the local metric $\tilde{M}_i$ for each point $x_i$
2: for $\text{iter} = 1$ to MAXITER do
3:   Estimate the density $p(x)$ for each point
4:   Compute the global metric $M = \sum_i p(x_i)\tilde{M}_i$
5:   Transform each point by $x_i \leftarrow Lx_i$, where $L^TL = M$
6: end for
7: Return $M$

B Linear combination of local metrics: other forms

The uniform combination eq. (11) and the resulting metric $M^\text{UNI}$, is a special case of convex combination of local metrics. Here, we consider another form of convex combination, where the combination coefficients (or weights) are proportional to the probabilistic density of each point. The densities are estimated by density estimators. Typically, a density estimator also depends on the metric used: a better metric can often lead to better estimation of densities. Thus we propose the iterative procedure listed in the Algorithm 1 to jointly estimate the densities and combine local metrics.

We have experimented with two types of density estimators:

- Kernel Density Estimator (KDE). Given the training data $\{x_1, ..., x_n\}$, the density of a testing point $x_t$ is defined as $p(x_t) = 1/h \sum_{i=1}^{n} \exp(-\|x_t - x_i\|^2/\sigma^2)$, where $h$ is a normalization constant, and $\sigma$ is the bandwidth parameter which is tuned on the validation data (to maximize the likelihood).

- Gaussian Mixture Model (GMM). The model is built by modeling each class as a single Gaussian. Note that the densities calculated from GMM are metric invariant if the class assignments are fixed. To make the density metric-dependent, we use the following trick: once the global metric is learnt, we use it to re-classify all training data (by kNN) based on the validation data. After that, we build GMM according to the new labels, and reiterate the process.

C Experimental details on metric learning for supervised learning tasks

C.1 Linear combination of local metrics

We compare eight metric learning methods, including two new methods described in Section B:

- Euclidean. We use the identity matrix as a metric to compute distances.
- LMNN. We learn a single metric discriminatively using the large margin nearest neighbor method [5], as reviewed in section 2.
- GLM$^{\text{INT}}$. We learn local metrics using generative techniques [11], as reviewed in section 2. We use Gaussian distributions as the class conditional distributions for our generative modeling. We follow the procedure defined in [11] to interpolate the learned local metrics with the Euclidean metric when we classify new data points. We do not report the results of un-interpolated metrics GLMs as our findings are consistent with the authors of [11]. The interpolated metrics have much better performance.
- $M^\text{UNI}$. This is our approach of combining the un-interpolated GLMs into a single metric with the uniform combination, described in eq. (11) of section 3.1.
- LMNN$_E$. With the same metric of LMNN, this method performs energy-based classification [5]. Loosely speaking, the energy of a point being assigned to a class $c$ is defined as the differences between two quantities: the (sum of) distances of this point to its nearest neighbor in class $c$ and the (sum of) distances of this point to its nearest neighbor in classes other than $c$. A point is assigned to the class which has the lowest energy. According to [5], energy-based classification sometimes improve performance significantly over purely nearest-neighbor based classification.
- $M^\text{GMM}$. Learn the global metric as a weighted combination of local metrics. The weight is proportional to the density estimated from Gaussian Mixture Model. The number of iterations in the Algorithm 1 is set to 20.
Table 4: Error rates of misclassification (in %) on small-scale datasets

| METHOD | DATASET  | 3-Normal | Wine  | Iris  | Heart  |
|--------|----------|----------|-------|-------|--------|
| Euclidean | 8.17 ± 0.33 | 4.41 ± 0.61 | 5.11 ± 0.69 | 22.78 ± 0.88 |
| LMNN   | 4.70 ± 0.30 | 2.61 ± 0.38 | 4.78 ± 0.71 | 21.91 ± 0.84 |
| GLM    | 3.83 ± 0.18 | 3.96 ± 0.64 | 3.67 ± 0.54 | 21.60 ± 0.92 |
| M UNI  | 3.44 ± 0.25 | 1.80 ± 0.40 | 3.33 ± 0.48 | 19.51 ± 0.90 |
| M GMM  | 2.96 ± 0.21 | 2.97 ± 0.51 | 3.44 ± 0.54 | 20.56 ± 0.80 |
| M KDE  | 3.70 ± 0.24 | 2.43 ± 0.44 | 4.67 ± 0.54 | 19.26 ± 0.76 |
| M UNI E| 3.10 ± 0.23 | 2.52 ± 0.52 | 3.11 ± 0.57 | 19.26 ± 0.76 |

| METHOD | DATASET  | Vehicle | Ionosphere | Image | German  |
|--------|----------|---------|------------|-------|---------|
| Euclidean | 31.29 ± 0.54 | 15.87 ± 0.68 | 2.68 ± 0.13 | 27.27 ± 0.60 |
| LMNN   | 25.32 ± 0.65 | 6.24 ± 0.52 | 2.14 ± 0.12 | 27.20 ± 0.58 |
| GLM INT| 17.47 ± 0.30 | 9.67 ± 0.48 | 2.47 ± 0.13 | 26.12 ± 0.62 |
| M UNI  | 18.15 ± 0.49 | 9.77 ± 0.49 | 2.27 ± 0.10 | 25.87 ± 0.68 |
| M GMM  | 17.17 ± 0.33 | 9.01 ± 0.49 | 2.12 ± 0.12 | 26.10 ± 0.66 |
| M KDE  | 20.37 ± 0.52 | 11.97 ± 0.66 | 2.67 ± 0.13 | 26.88 ± 0.55 |
| M UNI E| 15.81 ± 0.52 | 10.80 ± 0.71 | 3.01 ± 0.16 | 25.15 ± 0.51 |

- $M^{KDE}$. Learn the global metric as a weighted combination of local metrics. The weight is proportional to the density estimated from (Gaussian) Kernel Density Estimator. The number of iterations in the Algorithm 1 is set to 20.

For energy-based classification, we need to set a quantity called “margin” $\gamma_0$. We have used the follow procedure:

- transform all samples by the learnt metric.
- for each sample, compute the difference from: a) the distance to its nearest neighbor in the same class; b) the distance to its nearest neighbor in other classes.
- compute the median of these differences and denote its value as $\gamma_0$. Consider $\beta \gamma_0$ as candidate margins, where $\beta$ is a scaling factor tuned on validation set.

The error rates (mean and standard error) on small-scale datasets are listed in Table 4 with ranking information shown in Table 5. We can see that on most datasets, $M^{UNI}$ and $M^{UNI}_E$ outperform GLM INT, LMNN, LMNN E and Euclidean. Additionally, $M^{KDE}$ performs better than $M^{UNI}$, $M^{UNI}_E$ and $M^{GMM}$ in general. However, $M^{KDE}$ is less efficient than $M^{UNI}$ due to its iterative nature. We plan to explore more efficient and theoretical-sound combination approach in our future work.

The error rates (mean and standard error) on large-scale datasets are shown in Table 6. $M^{UNI}$ and $M^{UNI}_E$ generally performs well. In particular, with the low dimensionality of 40, $M^{UNI}_E$ reaches almost the same accuracy (error rate: 1.40%) as discriminatively trained metrics (LMNN) at a higher dimensionality of 164 (error rate: 1.34%).

C.1.1 Training speed

The training time of LMNN and $M^{UNI}$ on small-scale and large-scale datasets are given in Table 7 and 8, respectively. Note that the time reported here is the training time per tuning (i.e. run once with fixed parameters), which does not count the time for parameter-tuning (required in LMNN). Clearly, on most datasets, $M^{UNI}$ achieves one or two-order-magnitude speedup over LMNN. It is also interesting to point out that the scale of features may affect the training time of LMNN significantly (LMNN runs faster on Letters-original than Letters-scaled), as it can change the number of active constraints.
### Table 5: Ranking of different methods

| METHOD  | DATASET  | Avg. | Rank |
|---------|----------|------|------|
| Euclidean | Iris     | 8    | 7.75 |
|          | Wine     | 8    | 5    |
|          | Heart    | 8    | 5    |
|          | Vehi.    | 8    | 5    |
|          | Ionos.   | 6    | 5    |
|          | Image    | 6    | 5    |
|          | German   | 8    | 5    |
| LMNN     | Iris     | 7    | 6    |
|          | Wine     | 5    | 6    |
|          | Heart    | 7    | 6    |
|          | Vehi.    | 7    | 6    |
|          | Ionos.   | 2    | 6    |
|          | Image    | 7    | 6    |
|          | German   | 7    | 6    |
| GLM     | Iris     | 6    | 5    |
|          | Wine     | 7    | 5    |
|          | Heart    | 6    | 5    |
|          | Vehi.    | 7    | 5    |
|          | Ionos.   | 1    | 5    |
|          | Image    | 7    | 5    |
|          | German   | 7    | 5    |
|\(M_{\text{UNI}}\) | Iris     | 4    | 4    |
|          | Wine     | 1    | 4    |
|          | Heart    | 2    | 4    |
|          | Vehi.    | 3    | 4    |
|          | Ionos.   | 3    | 4    |
|          | Image    | 3    | 4    |
|          | German   | 4    | 4    |
|\(M_{\text{KDE}}\) | Iris     | 1    | 3    |
|          | Wine     | 6    | 3    |
|          | Heart    | 4    | 3    |
|          | Vehi.    | 4    | 3    |
|          | Ionos.   | 4    | 3    |
|          | Image    | 4    | 3    |
|          | German   | 4    | 3    |
| LMNN\(_E\) | Iris     | 5    | 2    |
|          | Wine     | 3    | 2    |
|          | Heart    | 6    | 2    |
|          | Vehi.    | 5    | 2    |
|          | Ionos.   | 6    | 2    |
|          | Image    | 5    | 2    |
|          | German   | 6    | 2    |
|\(M_{\text{UNI}}\)\(_E\) | Iris     | 3    | 1    |
|          | Wine     | 4    | 1    |
|          | Heart    | 1    | 1    |
|          | Vehi.    | 5    | 1    |
|          | Ionos.   | 8    | 1    |
|          | Image    | 1    | 1    |
|          | German   | 8    | 1    |

### Table 6: Error rates of misclassification (in %) on large-scale datasets

| METHOD  | DATASET  | ERROR RATE |
|---------|----------|------------|
| Euclidean | MNIST-40 | 2.09 ± 0.02 |
|          | MNIST-60 | 2.02 ± 0.02 |
|          | MNIST-164| 2.16 ± 0.01 |
|          | Letters-scaled | 5.05 ± 0.07 |
|          | Letters-original | 5.25 ± 0.08 |
| LMNN     | MNIST-40 | 1.99 ± 0.03 |
|          | MNIST-60 | 1.84 ± 0.01 |
|          | MNIST-164| 1.82 ± 0.01 |
|          | Letters-scaled | 3.91 ± 0.08 |
|          | Letters-original | 3.81 ± 0.13 |
| GLM     | MNIST-40 | 3.75 ± 0.06 |
|          | MNIST-60 | 3.55 ± 0.05 |
|          | MNIST-164| 3.48 ± 0.09 |
|          | Letters-scaled | 5.55 ± 0.08 |
|          | Letters-original | 5.51 ± 0.08 |
|\(M_{\text{UNI}}\) | MNIST-40 | 1.93 ± 0.03 |
|          | MNIST-60 | 1.90 ± 0.03 |
|          | MNIST-164| 4.30 ± 0.04 |
|          | Letters-scaled | 3.04 ± 0.08 |
|          | Letters-original | 2.96 ± 0.09 |
| LMNN\(_E\) | MNIST-40 | 1.53 ± 0.01 |
|          | MNIST-60 | 1.43 ± 0.01 |
|          | MNIST-164| 1.34 ± 0.01 |
|          | Letters-scaled | 2.98 ± 0.06 |
|          | Letters-original | 2.90 ± 0.06 |
|\(M_{\text{UNI}}\)\(_E\) | MNIST-40 | 1.40 ± 0.01 |
|          | MNIST-60 | 1.44 ± 0.01 |
|          | MNIST-164| 3.13 ± 0.03 |
|          | Letters-scaled | 2.26 ± 0.04 |
|          | Letters-original | 2.28 ± 0.06 |

### C.2 Nonlinear combination of local metrics

We learn the nonlinear combination of metrics in the framework of convex combination of nonlinear kernels [13, 23]. Our baseline systems learn a kernel in the following form

\[ K(x, x') = \sum \alpha_l \exp\left\{-\tau_l \|x - x'\|_2^2 / \sigma_0^2 \right\} \quad (24) \]

where \(\alpha_l\) represents coefficients of convex combination, \(\sigma_0^2\) is a normalization factor to fix the scale of the kernel. The “scaled” (inverse) bandwidth \(\tau_l\) takes values from \([2^{-6}, 2^{-5}, \ldots, 2^7, 2^8]\).

For nonlinear combination of metrics, instead of using all local metrics, we consider \(P\) “regional” metrics for the sake of computational efficiency (the regional metrics are obtained by averaging the local metrics in each cluster). We then use those regional metrics to compose the desired kernel with the formulation of eq. (13). We use the same scaling scheme for constructing the baseline eq. (24) and adjust \(\sigma_0^2\) accordingly (with respect to each different regional metric).

The combination coefficients are learnt in the framework of SimpleMKL [23], which minimizes the empirical risk of the support vector machines (SVM). For simplicity, let us denote the combined kernel as \(\sum \alpha_i K_i\), where \(\{K_i\}\) refers to the set of base kernels. SimpleMKL essentially solves the following optimization problem for binary classification (can be extended for multi-way classification using one-against-all or one-against-one approaches):

\[
\min_{\alpha} \max_{\beta} \quad \beta^T e - \frac{1}{2} \beta^T \left( \sum \alpha_i K_i \right) \beta \quad (25)
\]

subject to \(\beta \geq 0, \beta^T y = 0; \alpha \geq 0, \alpha^T e = 0\) \quad (26)

where \(\beta\) is the vector containing SVM dual variables, and \(e\) refers to all-one vectors.

The SimpleMKL is an iterative numerical optimization procedure to optimize the kernel combining coefficients \(\alpha_i\). The amount of time in finding the optimal solution depends on many factors including the number of base kernels. Thus, its computational cost can be substantive. In this aspect, we view \(M_{\text{UNI}}\), ie, simply averaging local metrics, as a strong contender in both improving performance and computational efficiency.
Table 7: Training time per tuning (seconds) on small-scale datasets

|          | 3-Norm. | Wine | Iris | Heart | Vehi. | Ionos. | Image | German |
|----------|---------|------|------|-------|-------|--------|-------|--------|
| LMNN     | 195.3   | 1.9  | 3.5  | 3.2   | 126.6 | 12.1   | 160.7 | 8.2    |
| $M^{\text{UNI}}$ | 0.3     | 0.03 | 0.04 | 0.06  | 0.5   | 0.3    | 0.8   | 0.3    |

Table 8: Training time per tuning (minutes) on large-scale datasets

|          | MNIST-40 | MNIST-60 | MNIST-164 | Letters-scaled | Letters-original |
|----------|----------|----------|------------|----------------|-----------------|
| LMNN     | 42       | 55       | 215        | 14             | 3               |
| $M^{\text{UNI}}$ | 4        | 7        | 47         | 1              | 1               |

The results on misclassification error rates are shown in Table 9 where Local (P) denotes our nonlinear combination method with P regional metrics. Out of 7 datasets we have experimented, nonlinear combination of metrics often outperform the baseline, with significant improvement on the datasets of 3-Normal, Iris and Vehicle. We observe that although nonlinear combining local metrics is promising, choosing the right number of local kernels is important. (It is often impractical to combine local kernels defined on all data points due to the heavy computational cost.)

D Application to unsupervised learning

Many unsupervised learning problems, such as clustering and dimensionality reduction, also depend on using a proper metric to calculate distances. We investigate how to apply the supervised metric learning algorithms to such problems. The crucial step is to extract labels for the algorithms to compute better metrics.

In unsupervised clustering, we start with k-means clustering with the Euclidean distance metric. We then treat the cluster labels as if they are ground-truth class labels. We apply the generative metric learning algorithm to such “labeled” data, compute local metrics and then global metric. We then apply k-means clustering again using the learnt global metric to compute distances. We iterate the process for a few times or until the cluster labels no longer change. Our empirical study shows that this simple strategy works well. The algorithm returns with clustering of higher quality, measured in standard measures, than k-means. Note that being able to have a global metric is essential. Without it, it is difficult to compare distances measured in different (local) metrics.

We demonstrate the usage of our global metric in the clustering problem. We use the small-scale datasets in the previous section, and try k-means clustering with the metric from $M^{\text{UNI}}$, as well as with the standard Euclidean metric. We set the $k$ equal to the number of classes, and iteratively obtain labels and metrics, as described previously.

The clustering results are measured by the RAND score. It is a similarity measure between two label sets, where the maximum 1 indicates the two labels sets show the exactly same clustering results. We calculate the RAND score based on the cluster assignment returned by k-means and the true labels of these datasets.

We set the $k$ equal to the number of classes, and iteratively obtain labels and metrics, as described previously.

The clustering results are measured by the RAND score. It is a similarity measure between two label sets, where the maximum 1 indicates the two labels sets show the exactly same clustering results. We calculate the RAND score based on the cluster assignment returned by k-means and the true labels of these datasets.

For unsupervised learning, we find that it is useful to regularize covariance matrices and interpolate local metrics, before computing the global metric. Indeed, regularization and interpolation can prevent overfitting, and generally lead to better clustering results. To tune these parameters, we split each dataset into a training, validation and testing set by the ratio of 60/20/20. We adopt the following procedure for parameter tuning: for each parameter combination, learn clusters on the training set, and use the clusters to cluster the validation set. Then, we compute the RAND score on the validation set to measure the performance of current parameter combination. Finally, we use the best tuned parameter combination to learn the clusters on the training set, and use them to cluster the testing set. We report the RAND score on the testing set as an indicator of the model performance.

Table 10 gives the RAND scores of different methods, averaged over 30 splits. We find that k-means + $M^{\text{UNI}}$ performs better than k-means + Euclidean on 5 (out of 8) datasets, with significant improvement on Iris and Image datasets. However, metric learning can also have negative effect, as revealed on Heart and Wine datasets.
Table 9: Error rates of misclassification (in %) with nonlinear combination of metrics

| METHOD               | DATASET | 3-Normal | Wine | Iris | Heart |
|----------------------|---------|----------|------|------|-------|
| Baseline             | 6.08 ± 0.27 | 2.16 ± 0.40 | 5.56 ± 0.65 | 18.09 ± 0.71 |
| Local (P = 1)        | 3.36 ± 0.26 | 2.43 ± 0.49 | 3.33 ± 0.60 | 17.16 ± 0.57 |
| Local (P = 5)        | 2.72 ± 0.26 | 4.14 ± 0.56 | 2.78 ± 0.36 | 19.26 ± 0.82 |
| Local (P = 10)       | 2.31 ± 0.24 | 3.96 ± 0.70 | 2.89 ± 0.47 | 18.95 ± 0.79 |

| METHOD               | DATASET | Vehi. | Ionos. | German |
|----------------------|---------|-------|--------|--------|
| Baseline             | 26.53 ± 0.53 | 6.90 ± 0.43 | 25.22 ± 0.38 |
| Local (P = 1)        | 15.36 ± 0.45 | 9.01 ± 0.58 | 24.38 ± 0.44 |
| Local (P = 5)        | 15.44 ± 0.42 | 10.47 ± 0.65 | 24.30 ± 0.42 |
| Local (P = 10)       | 15.58 ± 0.47 | 9.81 ± 0.53 | 24.25 ± 0.40 |

Table 10: RAND score on small-scale datasets

| METHOD               | DATASET | 3-Normal | Iris | Wine | Heart |
|----------------------|---------|----------|------|------|-------|
| k-means+Euclidean    | 0.528 ± 0.003 | 0.878 ± 0.009 | 0.935 ± 0.008 | 0.654 ± 0.008 |
| k-means+M^UNT        | **0.545** ± 0.008 | **0.948** ± 0.006 | 0.930 ± 0.008 | 0.643 ± 0.007 |

| METHOD               | DATASET | Vehi. | Ionos. | Image | German |
|----------------------|---------|-------|--------|-------|--------|
| k-means+Euclidean    | 0.651 ± 0.001 | 0.565 ± 0.007 | 0.510 ± 0.002 | 0.500 ± 0.0005 |
| k-means+M^UNT        | **0.657** ± 0.002 | **0.569** ± 0.008 | **0.567** ± 0.006 | 0.500 ± 0.0005 |