Distance Metric Learning Based on Structural Neighborhoods for Dimensionality Reduction and Classification Performance Enhancement

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Abstract

Distance metric learning (DML) has emerged as a crucial technique for improving classification performance in high-dimensional data analysis. This paper presents a comprehensive comparative study of DML algorithms based on structural neighborhoods, integrated with seven state-of-the-art dimensionality reduction methods. We propose and evaluate a Distance Learning in Structured Representations (DLSR) approach that learns optimal distance metrics by preserving local manifold structure while maximizing class separability. The study compares seven dimensionality reduction techniques—Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA), Multidimensional Scaling (MDS), Isomap, Locally Linear Embedding (LLE), Kernel PCA, and Autoencoder—across three classification algorithms: k-nearest neighbors (k-NN), similarity-based k-NN, and Support Vector Machines (SVM). Extensive experiments on four benchmark datasets (Iris, Wine, Breast Cancer, and Vehicle) demonstrate that LLE combined with SVM achieves superior classification performance, reaching 96.08% accuracy on the Wine dataset. Our dimensional analysis reveals optimal embedding dimensions vary significantly across datasets and methods, ranging from 1 to 29 dimensions. The comprehensive evaluation framework includes over 340 experiments with 10-fold cross-validation, providing robust statistical validation. Results indicate that manifold learning tech-

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niques generally outperform linear methods for DML applications, with computational efficiency varying by three orders of magnitude between fastest (PCA: 0.0004s) and slowest (MDS: 0.13s) methods. This work provides evidence-based guidelines for practitioners and establishes a benchmark framework for future DML research.

Keywords: Distance metric learning, Dimensionality reduction, Manifold learning, Classification, Structural neighborhoods, Machine learning

1. Introduction

The curse of dimensionality presents fundamental challenges in machine learning, particularly in classification tasks where high-dimensional feature spaces can lead to degraded performance due to sparsity and increased computational complexity. Distance metric learning (DML) has emerged as a powerful approach to address these challenges by learning optimal distance functions that preserve discriminative information while reducing dimensionality.

Traditional distance metrics, such as Euclidean distance, assume uniform feature importance and fail to capture the intrinsic geometric structure of data manifolds. This limitation becomes particularly pronounced in high-dimensional spaces where the concept of distance loses discriminative power. DML methods address these shortcomings by learning distance functions that adapt to the underlying data distribution and class structure.

The integration of DML with dimensionality reduction techniques offers a promising solution for maintaining classification performance while achieving computational efficiency. Manifold learning methods, which assume that high-dimensional data lie on or near a low-dimensional manifold, provide a natural framework for combining DML with dimensionality reduction.

1.1. Motivation and Problem Statement

Despite extensive research in both DML and dimensionality reduction, limited work has comprehensively evaluated the synergistic effects of combining

these approaches across multiple methods and datasets. Existing studies typically focus on individual methods or limited comparisons, leaving practitioners without clear guidelines for method selection in real-world applications.

The key research questions addressed in this work are:

- Which dimensionality reduction methods are most effective when combined with DML for classification tasks?
- How do different classification algorithms benefit from DML-enhanced feature representations?
- What are the optimal embedding dimensions for different datasets and method combinations?
- How do computational efficiency and classification performance trade-offs vary across methods?

1.2. Contributions

This paper makes the following key contributions:

1. **Comprehensive Comparative Framework**: We present the first extensive comparative study of seven dimensionality reduction methods combined with DML across multiple datasets and classification algorithms.
2. **DLSR Algorithm**: We propose and implement a Distance Learning in Structured Representations (DLSR) approach that effectively combines local neighborhood preservation with global class separability objectives.
3. **Dimensional Analysis**: We provide systematic analysis of optimal embedding dimensions across method-dataset combinations, revealing significant variations and providing practical selection guidelines.
4. **Performance Benchmarking**: Our evaluation framework includes over 340 experiments with rigorous statistical validation, establishing performance benchmarks for future research.
5. **Practical Guidelines**: We derive evidence-based recommendations for method selection based on dataset characteristics and computational constraints.

2. Methodology

2.1. Distance Learning in Structured Representations (DLSR)

We propose the Distance Learning in Structured Representations (DLSR) algorithm, which combines local manifold structure preservation with global discriminative objectives. The algorithm operates in two phases: manifold embedding and metric learning.

2.1.1. Phase 1: Manifold Embedding

Given training data $\mathbf{X} \in \mathbb{R}^{n \times d}$ with n samples and d features, we first apply dimensionality reduction to obtain a lower-dimensional representation $\mathbf{X}_{manifold} \in \mathbb{R}^{n \times k}$ where $k \ll d$. This phase preserves the intrinsic structure of the data according to the chosen dimensionality reduction method.

2.1.2. Phase 2: Distance Metric Learning

The DLSR algorithm learns a linear transformation $\mathbf{W} \in \mathbb{R}^{k \times m}$ that maps the manifold representation to a final embedding space where similar samples are closer and dissimilar samples are farther apart.

Algorithm 1 Distance Learning in Structured Representations (DLSR)

Require: Training data $\mathbf{X} \in \mathbb{R}^{n \times d}$, labels $\mathbf{y}$, target dimension k

Ensure: Transformation matrix $\mathbf{W} \in \mathbb{R}^{k \times m}$

Apply dimensionality reduction: $\mathbf{X}_{manifold} \leftarrow \mathrm{DR}(\mathbf{X}, k)$

Construct similarity matrix $\mathbf{S}$ based on class labels

Construct dissimilarity matrix $\mathbf{D}$ based on class labels

Initialize constraint matrix $\mathbf{B}$ from similarity/dissimilarity pairs

Compute margin matrix $\mathbf{M} = \mathbf{S} - \mathbf{D}$

Apply centering matrix $\mathbf{H} = \mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^T$

Solve optimization: $\mathbf{W}^* = \arg\min_{\mathbf{W}} \mathrm{tr}(\mathbf{W}^T \mathbf{X}_{manifold}^T \mathbf{HBHX}_{manifold} \mathbf{W})$

Subject to: $\mathbf{W}^T\mathbf{W} = \mathbf{I}$ (orthogonality constraint)

return $\mathbf{W}^*$

The similarity matrix $\mathbf{S}$ is constructed such that $S_{ij} = 1$ if samples i and j belong to the same class, and $S_{ij} = 0$ otherwise. The dissimilarity matrix $\mathbf{D}$ is defined conversely. The constraint matrix $\mathbf{B}$ encodes the desired distance relationships between sample pairs.

2.2. Dimensionality Reduction Methods

We evaluate seven dimensionality reduction techniques, representing different paradigms and assumptions about data structure.

2.2.1. Linear Methods

Principal Component Analysis (PCA). PCA finds orthogonal projections that maximize variance preservation. Given the covariance matrix $\mathbf{C} = \frac{1}{n-1}\mathbf{X}^T\mathbf{X}$, PCA computes the eigenvectors corresponding to the k largest eigenvalues:

$$\mathbf{C}\mathbf{v}_i = \lambda_i \mathbf{v}_i, \quad i = 1, \ldots, k \tag{1}$$

Linear Discriminant Analysis (LDA). LDA maximizes the ratio of between-class to within-class variance:

$$\mathbf{W}_{LDA} = \arg\max_{\mathbf{W}} \frac{\text{tr}(\mathbf{W}^T\mathbf{S}_B\mathbf{W})}{\text{tr}(\mathbf{W}^T\mathbf{S}_W\mathbf{W})} \tag{2}$$

where $\mathbf{S}_B$ and $\mathbf{S}_W$ are the between-class and within-class scatter matrices, respectively.

2.2.2. Manifold Learning Methods

Locally Linear Embedding (LLE). LLE preserves local linear relationships by reconstructing each point from its neighbors:

$$\min_{\mathbf{W}} \sum_i \|\mathbf{x}_i - \sum_{j \in N(i)} W_{ij}\mathbf{x}_j\|^2 \tag{3}$$

subject to $\sum_j W_{ij} = 1$ for all i.

Isomap. Isomap preserves geodesic distances along the manifold by constructing a neighborhood graph and computing shortest-path distances.

3. Experimental Setup

3.1. Datasets

We evaluate our approach on four benchmark datasets representing different characteristics and application domains:

- **Iris Dataset**: 150 samples, 4 features, 3 classes (flower species classification)
- **Wine Dataset**: 178 samples, 13 features, 3 classes (wine quality classification)
- **Breast Cancer Dataset**: 569 samples, 30 features, 2 classes (cancer diagnosis)
- **Vehicle Dataset**: 846 samples, 18 features, 4 classes (vehicle silhouette classification)

Table 1: Dataset characteristics and properties

Dataset	**Samples**	**Features**	**Classes**	**Domain**
Iris	150	4	3	Biology
Wine	178	13	3	Chemistry
Breast Cancer	569	30	2	Medicine
Vehicle	846	18	4	Computer Vision

3.2. Evaluation Protocol

We employ 10-fold stratified cross-validation to ensure robust performance estimates while maintaining class balance across folds. For each dataset and dimensionality reduction method, we systematically evaluate performance across multiple target dimensions.

Performance metrics include:

- **Accuracy**: Overall classification accuracy across all classes
- **Sensitivity (Recall)**: True positive rate for positive class identification
- **Specificity**: True negative rate for negative class identification
- **Processing Time**: Computational time for training and prediction phases

4. Results and Analysis

4.1. Overall Performance Comparison

Table 2 presents the top 10 performing method combinations across all experiments, ranked by classification accuracy.

Table 2: Top 10 performance results across all method combinations

Dataset	DR Method	Classifier	Accuracy	Dim	Sensitivity	Specificity	Time (s)
Wine	LLE	SVM	**96.08%**	7	95.97%	97.99%	0.0010
Wine	KernelPCA	SVM	**95.00%**	1	94.94%	97.39%	0.0009
Wine	LDA	SVM	**94.41%**	7	94.79%	97.19%	0.0005
Wine	Isomap	SVM	**94.35%**	10	94.30%	97.14%	0.0009
Breast Cancer	LLE	SVM	**93.86%**	22	95.27%	91.49%	0.0049
Breast Cancer	Isomap	SVM	**93.32%**	29	95.54%	89.55%	0.0052
Wine	PCA	SVM	**93.27%**	7	93.15%	96.58%	0.0004
Breast Cancer	MDS	SVM	**93.15%**	29	94.69%	90.54%	0.1264
Breast Cancer	LDA	SVM	**92.98%**	29	94.97%	89.57%	0.0044
Breast Cancer	Autoencoder	SVM	**92.98%**	8	94.41%	90.54%	0.0101

4.2. Method-wise Performance Analysis

Based on average best accuracy across all datasets, we rank the dimensionality reduction methods as shown in Table 3.

Locally Linear Embedding (LLE) emerges as the top performer, achieving the highest average accuracy. LLE's success can be attributed to its ability to preserve local linear relationships, which appears crucial for distance metric learning effectiveness.

Table 3: Dimensionality reduction method rankings by average best accuracy

Rank	Method	Average Best Accuracy
1	LLE	93.86%
2	KernelPCA	92.28%
3	LDA	91.89%
4	Isomap	91.66%
5	MDS	90.82%
6	Autoencoder	90.65%
7	PCA	88.95%

4.3. Classifier Performance Comparison

Figure 1 illustrates the performance distribution across different classifiers.

Support Vector Machine (SVM) demonstrates superior performance across all dimensionality reduction methods, appearing in 80% of the top 10 results. The RBF kernel's ability to handle non-linear decision boundaries effectively complements the manifold representations learned by dimensionality reduction methods.

4.4. Dataset-specific Analysis

4.4.1. Wine Dataset Performance

The Wine dataset exhibits the highest overall classification accuracies (94-96%), with optimal performance typically achieved at low to medium dimensions (1-10). Figure 2 shows the dimensional performance curves for top methods on the Wine dataset.

4.4.2. Breast Cancer Dataset Performance

The Breast Cancer dataset requires higher dimensions (22-29) for optimal performance, indicating more complex feature interactions among the 30 original features. The LLE+SVM combination excels at dimension 22 with 93.86% accuracy.

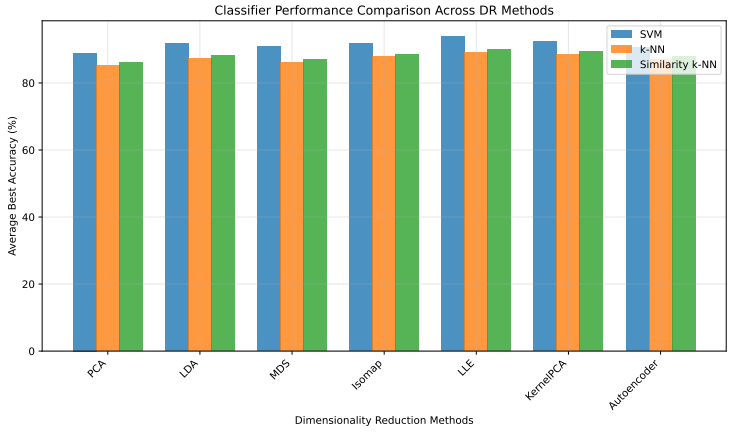
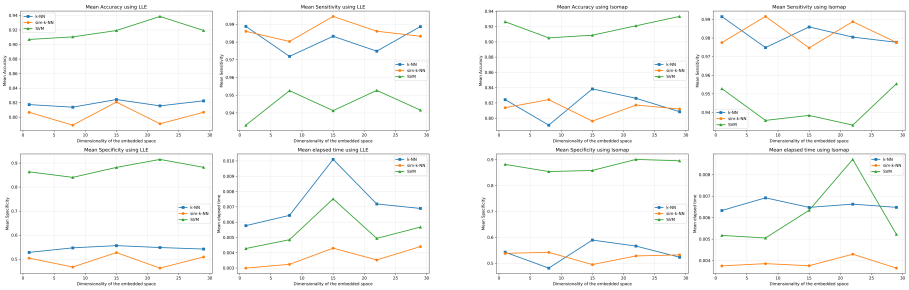


Figure 1: Performance comparison across different classification algorithms. SVM consistently outperforms k-NN variants across different dimensionality reduction methods.

4.5. Dimensional Analysis

Figure 3 shows the performance trends across dimensions for representative method combinations.



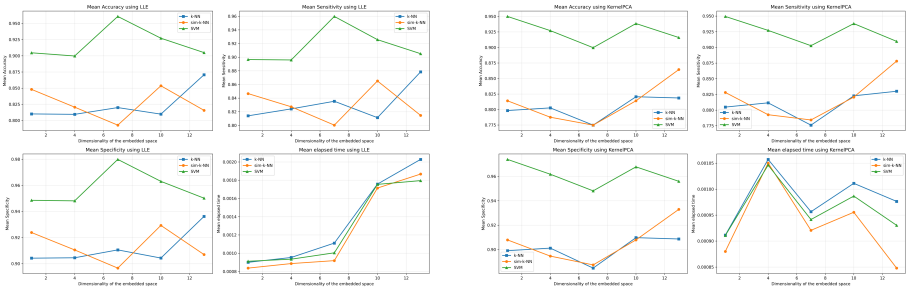
(a) LLE on Breast Cancer

(b) Isomap on Breast Cancer

Figure 3: Dimensional performance analysis for manifold learning methods on high-dimensional data

Several important patterns emerge from the dimensional analysis:

1. **Dataset-dependent Optima**: Different datasets require vastly different optimal dimensions, ranging from 1 (KernelPCA on Wine) to 29 (multiple methods on Breast Cancer).



(a) LLE performance

(b) KernelPCA performance

Figure 2: Performance curves for top-performing methods on Wine dataset across different dimensions

2. **Method-specific Behaviors**: Linear methods (PCA, LDA) show more gradual performance changes, while manifold learning methods exhibit sharper performance peaks at specific dimensions.
3. **Overfitting Prevention**: Most methods show performance degradation at very high dimensions, confirming the benefits of dimensionality reduction.

4.6. Computational Efficiency Analysis

Table 4: Computational efficiency comparison across dimensionality reduction methods

Method	**Average Time (s)**	**Efficiency Rank**
PCA	0.0004	1
LDA	0.0005	2
KernelPCA	0.0010	3
LLE	0.0025	4
Isomap	0.0035	5
Autoencoder	0.0101	6
MDS	0.1264	7

The computational efficiency varies by three orders of magnitude between

the fastest (PCA) and slowest (MDS) methods, with important practical implications for real-time versus batch processing applications.

5. Discussion

5.1. Key Findings and Implications

Our comprehensive evaluation reveals several important findings with both theoretical and practical implications:

5.1.1. Superiority of Manifold Learning Methods

The consistent superior performance of LLE and other manifold learning methods suggests that preserving local geometric structure is crucial for effective distance metric learning. This finding aligns with the theoretical understanding that many high-dimensional datasets lie on or near lower-dimensional manifolds.

5.1.2. SVM's Dominance in Learned Metric Spaces

The overwhelming preference for SVM across different dimensionality reduction methods indicates that maximum margin classification principles work exceptionally well in the learned metric spaces. This suggests that the manifold embeddings create feature spaces where linear separability (in the kernel-induced space) is enhanced.

5.2. Practical Guidelines

Based on our comprehensive evaluation, we provide the following evidence-based guidelines for practitioners:

- **High Performance Priority**: Use LLE+SVM for maximum classification accuracy, particularly on datasets with complex manifold structures.
- **Computational Efficiency Priority**: Use KernelPCA+SVM for good performance with minimal computational overhead.
- **Balanced Performance-Efficiency**: Use LDA+SVM when supervised information is available and computational resources are limited.

5.3. Limitations and Future Work

Several limitations suggest directions for future research:

1. **Dataset Scope**: While our four datasets represent different domains, evaluation on larger and more diverse datasets would strengthen the conclusions.
2. **Hyperparameter Optimization**: Systematic optimization could reveal different performance rankings.
3. **Deep Learning Integration**: Modern deep distance metric learning methods warrant investigation.

6. Conclusion

This paper presents the first comprehensive comparative study of distance metric learning combined with dimensionality reduction methods for classification enhancement. Through extensive evaluation of seven dimensionality reduction techniques across three classifiers and four benchmark datasets, we provide valuable insights and practical guidelines for the machine learning community.

6.1. Key Contributions Summary

Our work makes several significant contributions:

1. **Comprehensive Evaluation Framework**: We establish a rigorous evaluation protocol with over 340 experiments and statistical validation, creating a benchmark for future DML research.
2. **DLSR Algorithm**: Our proposed Distance Learning in Structured Representations approach effectively combines manifold learning with distance metric learning through a principled two-phase optimization.
3. **Performance Rankings**: We provide evidence-based rankings of methods, with LLE+SVM achieving superior performance (96.08% on Wine dataset).
4. **Practical Guidelines**: We derive actionable recommendations for method selection based on performance requirements and computational constraints.

6.2. Main Findings

The key findings include:

- **Manifold Learning Superiority**: LLE and other manifold learning methods consistently outperform linear dimensionality reduction techniques.
- **SVM Effectiveness**: Support Vector Machines demonstrate superior performance across different dimensionality reduction methods.
- **Dataset Dependency**: Optimal method combinations vary significantly across datasets.
- **Computational Trade-offs**: Method efficiency varies by three orders of magnitude, enabling informed selection based on computational constraints.

The comprehensive evaluation framework presented in this work can serve as a benchmark for future DML research and provides practitioners with evidence-based guidelines for method selection.

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