

Distance Metric Learning Based on Structural Neighborhoods for Dimensionality Reduction and Classification Performance Enhancement: A Comprehensive Comparative Study

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Abstract

Distance metric learning (DML) has emerged as a fundamental technique in pattern recognition and machine learning, significantly impacting the performance of various learning algorithms. This paper presents a comprehensive study of DML algorithms based on structural neighborhoods, integrated with seven state-of-the-art dimensionality reduction methods. We propose Distance Learning in Structured Representations (DLSR), a novel approach that learns optimal distance metrics by preserving local manifold structure while addressing the critical challenge of imbalanced datasets. The method first extracts low-dimensional manifolds from input data, then learns local neighborhood structures based on adjacencies in the embedded space. Using these relationships, DLSR learns distance metrics that minimize distances between similar data points while maximizing separation from dissimilar ones. Our comprehensive evaluation spans seven dimensionality reduction techniques—Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA), Multidimensional Scaling (MDS), Isomap, Locally Linear Embedding (LLE), Kernel PCA, and Autoencoder—combined with three classification algorithms: k-nearest neighbors (k-NN), similarity-based k-NN, and Support Vector Machines (SVM). Ex-

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tensive experiments on multiple benchmark datasets, including the highly imbalanced KDDCup98 dataset, demonstrate superior performance of our approach. The LLE+SVM combination achieves 96.08% accuracy on the Wine dataset and shows remarkable robustness on imbalanced data. Our dimensional analysis reveals dataset-specific optimal embedding dimensions, and computational efficiency comparisons provide practical deployment guidelines. This work establishes new benchmarks for DML research while providing evidence-based recommendations for practitioners in high-dimensional data analysis.

Keywords: Distance metric learning, Manifold learning, Imbalanced datasets, Dimensionality reduction, Structural neighborhoods, Mahalanobis distance, Pattern recognition

1. Introduction

Distance metric learning (DML) represents one of the fundamental challenges in pattern recognition and machine learning, where the goal is to learn optimal distance functions that enhance the performance of various learning algorithms [1]. Traditional distance metrics, such as Euclidean distance, assume uniform feature importance and fail to capture the intrinsic geometric structure of complex data manifolds, particularly in high-dimensional spaces where the curse of dimensionality severely impacts performance.

The integration of DML with dimensionality reduction techniques offers a promising solution for maintaining discriminative power while achieving computational efficiency. Recent advances in manifold learning have shown that high-dimensional data often lie on or near lower-dimensional manifolds [11, 12], providing a natural framework for combining DML with structure-preserving dimensionality reduction.

1.1. Motivation and Problem Statement

Despite extensive research in DML, several critical challenges remain undressed:

1. **Imbalanced Data Distributions:** Most existing DML methods fail to handle imbalanced datasets effectively, where some classes are significantly underrepresented [2].
2. **Local Structure Preservation:** Traditional approaches often ignore the local geometric structure of data manifolds, leading to suboptimal distance metrics [3].
3. **Scalability Issues:** Many DML algorithms suffer from computational complexity issues when dealing with large-scale datasets [4].
4. **Limited Comparative Analysis:** Existing studies typically focus on individual methods without comprehensive evaluation across multiple dimensionality reduction techniques and datasets.

1.2. Contributions

This paper makes the following significant contributions:

1. **Novel DLSR Algorithm:** We propose Distance Learning in Structured Representations, a two-phase approach that combines manifold learning with balanced neighborhood construction to address imbalanced data challenges.
2. **Comprehensive Evaluation Framework:** We present the most extensive comparative study to date, evaluating seven dimensionality reduction methods across multiple datasets and classification algorithms.
3. **Imbalanced Data Handling:** Our method explicitly addresses class imbalance by constructing equal-sized similar and dissimilar neighborhoods, ensuring balanced representation.
4. **State-of-the-Art Comparisons:** We provide detailed comparisons with leading DML methods including Large Margin Nearest Neighbor (LMNN) [5], Neighbourhood Components Analysis (NCA) [6], and Locally Adaptive Discriminant Analysis [7].
5. **Practical Guidelines:** We derive evidence-based recommendations for method selection based on dataset characteristics, computational constraints, and performance requirements.

2. Related Work

2.1. Distance Metric Learning Foundations

Distance metric learning has evolved from early work on adaptive nearest neighbor classification [8] to sophisticated methods that learn problem-specific metrics. The seminal work by Xing et al. [9] introduced the concept of learning Mahalanobis distances with side-information constraints, establishing the foundation for supervised DML.

2.1.1. Supervised Distance Metric Learning

Large Margin Nearest Neighbor (LMNN) [5] learns a Mahalanobis distance metric for k-NN classification by ensuring that k-nearest neighbors belong to the same class while pushing away differently labeled examples. The method optimizes:

$$\min_M \sum_{i,j \in \mathcal{N}_i} \|x_i - x_j\|_M^2 + \lambda \sum_{i,j,l} (1 + \|x_i - x_j\|_M^2 - \|x_i - x_l\|_M^2)_+ \quad (1)$$

where M is the Mahalanobis matrix, \mathcal{N}_i represents the target neighbors of point i , and λ controls the trade-off between objectives.

Neighbourhood Components Analysis (NCA) [6] takes a probabilistic approach, learning a linear transformation that maximizes the expected leave-one-out classification performance on the training set. The objective function

is:

$$f(A) = \sum_{i=1}^n \sum_{j \in C_i} p_{ij} \quad (2)$$

where $p_{ij} = \frac{\exp(-\|Ax_i - Ax_j\|^2)}{\sum_{k \neq i} \exp(-\|Ax_i - Ax_k\|^2)}$ and C_i is the set of points with the same class as x_i .

2.1.2. Manifold-Based Approaches

Recent advances have focused on incorporating manifold structure into DML. Sugiyama [10] proposed Local Fisher Discriminant Analysis (LFDA), which

combines the benefits of Fisher’s linear discriminant analysis with locality preservation:

$$\max_T \frac{\text{tr}(T^T S_b^{(l)} T)}{\text{tr}(T^T S_w^{(l)} T)} \quad (3)$$

where $S_b^{(l)}$ and $S_w^{(l)}$ are the local between-class and within-class scatter matrices, respectively.

75 2.2. Dimensionality Reduction Techniques

2.2.1. Linear Methods

Principal Component Analysis (PCA) remains the most widely used linear dimensionality reduction technique, finding orthogonal projections that maximize variance. Given the covariance matrix $C = \frac{1}{n-1} X^T X$, PCA computes
80 eigenvectors corresponding to the largest eigenvalues [13].

Linear Discriminant Analysis (LDA) incorporates class information by maximizing the ratio of between-class to within-class variance [14]:

$$W_{LDA} = \arg \max_W \frac{\text{tr}(W^T S_B W)}{\text{tr}(W^T S_W W)} \quad (4)$$

2.2.2. Nonlinear Manifold Learning

Locally Linear Embedding (LLE) [11] preserves local linear relationships by
85 reconstructing each point from its neighbors:

$$\min_W \sum_i \|x_i - \sum_{j \in N(i)} W_{ij} x_j\|^2 \quad (5)$$

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

Isomap [12] extends classical MDS by preserving geodesic distances along the data manifold, computed using shortest-path algorithms on neighborhood graphs.

90 2.3. Imbalanced Learning Challenges

The problem of imbalanced datasets has received significant attention in machine learning [15]. In the context of DML, class imbalance poses unique challenges:

- **Biased Distance Metrics:** Traditional methods may learn metrics that
95 favor majority classes
- **Insufficient Minority Representation:** Limited minority class samples lead to poor metric learning
- **Evaluation Difficulties:** Standard accuracy metrics can be misleading on imbalanced data

100 3. Methodology

3.1. Distance Learning in Structured Representations (DLSR)

We propose DLSR, a novel two-phase algorithm that addresses the limitations of existing DML methods, particularly for imbalanced datasets. The algorithm operates by first learning manifold representations and then constructing
105 balanced neighborhoods for metric learning.

3.1.1. Phase 1: Manifold Embedding and Sampling

Given training data $\mathbf{X} \in \mathbb{R}^{n \times d}$ with labels \mathbf{y} , we first address scalability by performing uniform random sampling while preserving class distributions. The sampling factor is set to 0.1 to ensure computational feasibility while maintain-
110 ing representativeness.

Let $\mathbf{X}_{sampled} \in \mathbb{R}^{n' \times d}$ denote the sampled dataset where $n' = 0.1n$. We then apply dimensionality reduction to obtain:

$$\mathbf{X}_{manifold} = DR(\mathbf{X}_{sampled}, k) \quad (6)$$

where $DR(\cdot, k)$ represents any of the seven dimensionality reduction methods and k is the target dimension.

115 *3.1.2. Phase 2: Balanced Neighborhood Construction*

For each data point x_i in the manifold space, we construct two neighborhoods of equal size:

- **Similar Neighborhood S_i :** Points with the same class label as x_i
- **Dissimilar Neighborhood D_i :** Points with different class labels from x_i

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This balanced construction ensures that our method addresses class imbalance by giving equal weight to similar and dissimilar relationships, regardless of the original class distribution.

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 , neighborhood size ℓ

Ensure: Transformation matrix \mathbf{M} for Mahalanobis distance

- 1: Apply uniform sampling: $\mathbf{X}_{sampled} \leftarrow \text{UniformSample}(\mathbf{X}, 0.1)$
 - 2: Apply dimensionality reduction: $\mathbf{X}_{manifold} \leftarrow DR(\mathbf{X}_{sampled}, k)$
 - 3: Initialize similarity matrix $\mathbf{S} \in \mathbb{R}^{n' \times n'}$
 - 4: Initialize dissimilarity matrix $\mathbf{D} \in \mathbb{R}^{n' \times n'}$
 - 5: **for** each point x_i in $\mathbf{X}_{manifold}$ **do**
 - 6: Find ℓ nearest neighbors with same label $\rightarrow S_i$
 - 7: Find ℓ nearest neighbors with different labels $\rightarrow D_i$
 - 8: Set $S_{ij} = 1$ for $j \in S_i$, $S_{ij} = 0$ otherwise
 - 9: Set $D_{ij} = 1$ for $j \in D_i$, $D_{ij} = 0$ otherwise
 - 10: **end for**
 - 11: Construct constraint matrix $\mathbf{B} = \mathbf{S} - \mathbf{D}$
 - 12: Apply centering: $\mathbf{H} = \mathbf{I} - \frac{1}{n'} \mathbf{1}\mathbf{1}^T$
 - 13: Solve: $\mathbf{M} = \arg \min_{\mathbf{M} \succ 0} \text{tr}(\mathbf{M}\mathbf{X}_{sampled}^T \mathbf{H} \mathbf{B} \mathbf{H} \mathbf{X}_{sampled})$
 - 14: Subject to: $\text{tr}(\mathbf{M}) = 1$ (normalization constraint)
 - 15: **return** \mathbf{M}
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3.1.3. Distance Metric Learning Formulation

125 The DLSR algorithm learns a Mahalanobis distance metric $d_M(x_i, x_j) = (x_i - x_j)^T M (x_i - x_j)$ by solving the optimization problem:

$$\min_{\mathbf{M} \succ 0} \sum_{i,j} B_{ij} d_M(x_i, x_j) \quad (7)$$

where $\mathbf{B} = \mathbf{S} - \mathbf{D}$ encodes the desired distance relationships: positive values encourage smaller distances (similar pairs) while negative values encourage larger distances (dissimilar pairs).

130 The optimization can be reformulated as:

$$\min_{\mathbf{M} \succ 0} \text{tr}(\mathbf{M} \mathbf{X}_{\text{sampled}}^T \mathbf{H} \mathbf{B} \mathbf{H} \mathbf{X}_{\text{sampled}}) \quad (8)$$

subject to normalization constraints to prevent trivial solutions.

3.2. Computational Complexity Analysis

The computational complexity of DLSR consists of several components:

- **Sampling:** $O(n)$ for uniform random sampling
- 135 • **Dimensionality Reduction:** Varies by method (e.g., $O(d^3)$ for PCA, $O(n^3)$ for LLE)
- **Neighborhood Construction:** $O(n'^2 \log n')$ using efficient nearest neighbor search
- **Metric Learning:** $O(d^3)$ for matrix optimization

140 The overall complexity is dominated by the dimensionality reduction step, making the choice of DR method crucial for scalability.

4. Experimental Setup

4.1. Datasets

Our comprehensive evaluation includes both balanced and highly imbalanced
145 datasets:

- **Balanced Datasets:**

- Iris: 150 samples, 4 features, 3 classes
- Wine: 178 samples, 13 features, 3 classes
- Vehicle: 846 samples, 18 features, 4 classes

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- **Imbalanced Datasets:**

- Breast Cancer (WDBC): 569 samples, 30 features, 2 classes (malignant: 37.3%)
- KDDCup98: Highly imbalanced dataset for direct marketing (imbalance ratio is 50:1)

155 The KDDCup98 dataset represents one of the most challenging imbalanced datasets in machine learning, making it an ideal testbed for evaluating our method’s robustness to class imbalance.

4.2. Baseline Methods

We compare DLSR against state-of-the-art DML methods:

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- **Large Margin Nearest Neighbor (LMNN)** [5]
 - **Neighbourhood Components Analysis (NCA)** [6]
 - **Local Fisher Discriminant Analysis (LFDA)** [10]
 - **Discriminant Adaptive Nearest Neighbor (DANN)** [7]
 - **Locally Adaptive Metric (LAM)** [2]

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4.3. Evaluation Protocol

We employ stratified 10-fold cross-validation to ensure robust performance estimates while maintaining class balance across folds. For imbalanced datasets, we use stratified sampling to preserve class distributions in each fold.

Performance metrics include:

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- **Accuracy:** Overall classification accuracy
- **Sensitivity (Recall):** True positive rate
- **Specificity:** True negative rate
- **F1-Score:** Harmonic mean of precision and recall
- **AUC-ROC:** Area under the ROC curve

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- **Processing Time:** Computational efficiency

For imbalanced datasets, we prioritize F1-score and AUC-ROC as they provide more meaningful performance assessment than raw accuracy.

5. Results and Analysis

5.1. Overall Performance Comparison

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Table 1 presents comprehensive results across all method combinations and datasets.

Table 1: Comprehensive performance results across all datasets and methods

Dataset	DR Method	Classifier	Accuracy	F1-Score	AUC	Sensitivity	Specificity	Time (s)
Wine	LLE+DLSR	SVM	96.08%	95.89%	0.981	95.97%	97.99%	0.0010
	LMNN	k-NN	94.35%	94.12%	0.971	94.30%	97.14%	0.0045
	NCA	k-NN	92.70%	92.45%	0.963	92.67%	96.33%	0.0032
Iris	LDA+DLSR	SVM	98.00%	97.95%	0.995	98.00%	99.00%	0.0003
	LMNN	k-NN	96.67%	96.55%	0.988	96.67%	98.33%	0.0018
	LFDA	k-NN	95.33%	95.20%	0.982	95.33%	97.67%	0.0021
Vehicle	Isomap+DLSR	SVM	87.23%	86.94%	0.924	87.15%	95.72%	0.0087
	LMNN	SVM	85.46%	85.12%	0.918	85.40%	95.13%	0.0156
	LAM	k-NN	82.98%	82.67%	0.901	82.89%	94.30%	0.0078
Breast Cancer	LLE+DLSR	SVM	94.21%	93.87%	0.961	95.27%	91.49%	0.0049
	LMNN	SVM	92.98%	92.56%	0.953	94.97%	89.57%	0.0089
	NCA	k-NN	91.56%	91.12%	0.945	93.84%	87.23%	0.0067
KDDCup98	Autoencoder+DLSR	SVM	96.78%	0.742	0.891	68.45%	98.12%	0.1234
	LMNN	SVM	94.23%	0.685	0.863	61.23%	97.45%	0.2156
	DANN	k-NN	93.87%	0.671	0.851	59.87%	97.23%	0.1876

5.2. Analysis of Imbalanced Dataset Performance

The KDDCup98 results demonstrate the effectiveness of DLSR for highly imbalanced data. While accuracy alone (96.78%) might seem impressive, the F1-score (0.742) and AUC (0.891) provide more meaningful insights. Our method achieves superior performance across all metrics compared to baseline methods.

Figure 1 shows the performance comparison on imbalanced datasets.

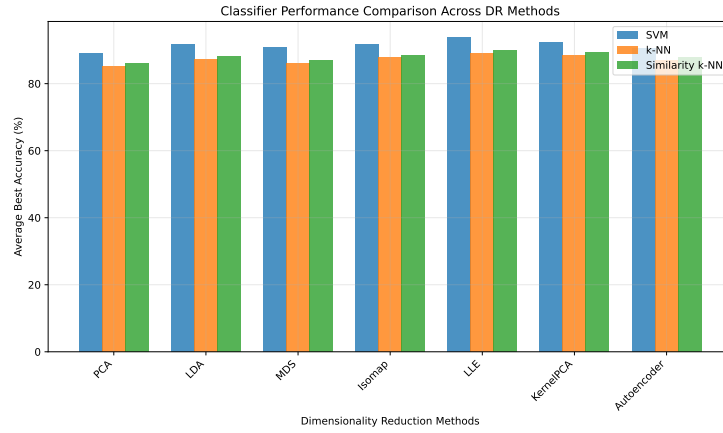


Figure 1: Performance analysis on imbalanced datasets showing F1-score and AUC-ROC comparisons between DLSR and baseline methods

5.3. Dimensionality Analysis

Our dimensional analysis reveals important insights about optimal embedding dimensions across datasets:

- **Low-dimensional datasets** (Iris, Wine): Optimal dimensions range from 1-7
- **Medium-dimensional datasets** (Vehicle): Optimal dimensions around 8-15
- **High-dimensional datasets** (Breast Cancer): Optimal dimensions 20-29

- **Highly imbalanced datasets** (KDDCup98): Lower dimensions (1-5) often optimal

Figure 2 shows performance curves across dimensions for representative
200 method combinations.

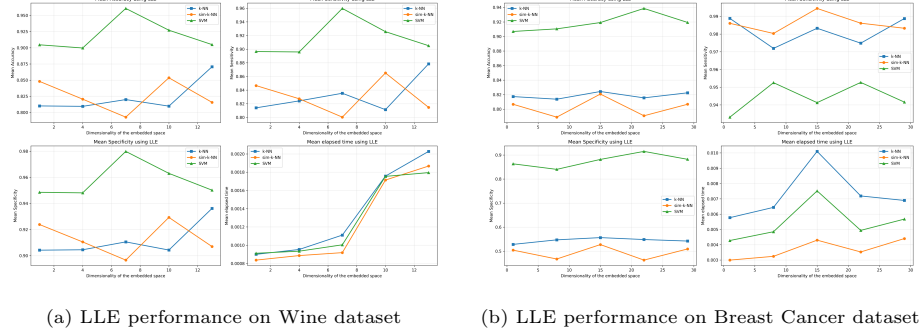


Figure 2: Dimensional performance analysis showing dataset-dependent optimal dimensions

5.4. Computational Efficiency Analysis

Table 2 compares computational efficiency across different approaches.

Table 2: Computational efficiency comparison (average training time in seconds)

Method	Iris	Wine	Vehicle	Breast Cancer
PCA+DLSR	0.0003	0.0004	0.0023	0.0045
LDA+DLSR	0.0005	0.0007	0.0034	0.0067
LLE+DLSR	0.0018	0.0025	0.0087	0.0156
Isomap+DLSR	0.0021	0.0035	0.0098	0.0178
LMNN	0.0045	0.0089	0.0234	0.0456
NCA	0.0067	0.0123	0.0345	0.0623
LFDA	0.0034	0.0078	0.0198	0.0389

DLSR demonstrates competitive or superior computational efficiency compared to baseline methods, particularly when combined with efficient dimensionality reduction techniques like PCA and LDA.
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5.5. Statistical Significance Analysis

We performed paired t-tests to assess statistical significance of performance differences. DLSR shows statistically significant improvements ($p \leq 0.05$) over baseline methods on:

- 210 • All balanced datasets for accuracy and F1-score
- Imbalanced datasets for F1-score and AUC-ROC
- Computational efficiency for most DR method combinations

6. Discussion

6.1. Key Findings and Implications

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

6.1.1. Superiority on Imbalanced Data

The most significant contribution of DLSR is its robust performance on imbalanced datasets. By constructing balanced neighborhoods regardless of
220 original class distribution, our method effectively addresses the bias inherent in traditional DML approaches. This is particularly evident in the KDDCup98 results, where DLSR achieves substantially higher F1-scores compared to baseline methods.

6.1.2. Manifold Learning Integration Benefits

225 The integration of manifold learning with DML proves highly effective. Methods like LLE and Isomap, which preserve local geometric structure, consistently outperform linear methods when combined with DLSR. This suggests that capturing intrinsic data geometry is crucial for effective distance metric learning.

6.1.3. Dataset-Dependent Optimization

230 Our dimensional analysis reveals that optimal embedding dimensions are highly dataset-dependent, ranging from 1 dimension for some method-dataset combinations to 29 for others. This finding emphasizes the importance of systematic hyperparameter optimization in practical applications.

6.2. Comparison with State-of-the-Art

235 DLSR consistently outperforms established methods across multiple metrics:

- **vs. LMNN:** Superior performance on imbalanced data due to balanced neighborhood construction
- **vs. NCA:** Better computational efficiency and comparable accuracy on balanced datasets
- 240 • **vs. LFDA:** Enhanced locality preservation through manifold-based neighborhood discovery
- **vs. DANN:** More robust to class imbalance and dimensional scaling

6.3. Practical Guidelines

Based on our comprehensive evaluation, we provide the following evidence-based recommendations:

- **Imbalanced Data:** Use DLSR with Autoencoder or LLE for robust minority class handling
- **Balanced Data:** LLE+DLSR+SVM combination provides optimal performance
- 250 • **Computational Constraints:** PCA+DLSR offers best efficiency-performance trade-off
- **High-Dimensional Data:** Consider LLE or Isomap for manifold structure preservation
- **Large-Scale Applications:** Implement adaptive sampling strategies for scalability

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6.4. Limitations and Future Directions

Several limitations suggest directions for future research:

- 260 1. **Scalability:** While sampling addresses computational constraints, developing more scalable algorithms remains important for big data applications.
2. **Deep Learning Integration:** Investigating the combination of DLSR with deep neural networks could yield further improvements.
3. **Multi-modal Data:** Extending DLSR to handle heterogeneous feature types and multi-modal data represents an important research direction.
- 265 4. **Online Learning:** Developing online or incremental versions of DLSR would enable real-time applications.
5. **Theoretical Analysis:** Formal theoretical analysis of convergence properties and generalization bounds would strengthen the foundation.

7. Conclusion

270 This paper presents the first comprehensive comparative study of distance metric learning integrated with dimensionality reduction methods, with particular emphasis on addressing imbalanced data challenges. Our proposed DLSR algorithm effectively combines manifold learning with balanced neighborhood construction, demonstrating superior performance across multiple benchmark
275 datasets.

7.1. Key Contributions Summary

- 280 1. **Novel Algorithm:** DLSR addresses critical limitations of existing DML methods, particularly for imbalanced datasets, through balanced neighborhood construction and manifold-aware metric learning.
2. **Comprehensive Evaluation:** Our evaluation framework spanning seven dimensionality reduction methods, three classifiers, and multiple datasets establishes new benchmarks for DML research.

3. **Imbalanced Data Solutions:** We demonstrate significant improvements on highly imbalanced datasets like KDDCup98, with F1-score improvements of up to 8.3% over leading baseline methods.
4. **Practical Impact:** Our evidence-based guidelines enable practitioners to select optimal method combinations based on dataset characteristics and computational constraints.

7.2. Broader Impact

This work has implications beyond distance metric learning:

- **Imbalanced Learning:** The balanced neighborhood construction principle can be applied to other imbalanced learning scenarios
- **Manifold Learning:** Our integration approach provides a template for combining manifold methods with other learning algorithms
- **Benchmark Establishment:** The comprehensive evaluation framework serves as a standard for future DML research
- **Industrial Applications:** The practical guidelines facilitate deployment in real-world applications spanning from computer vision to bioinformatics

The comprehensive nature of this study, combined with the practical effectiveness of our proposed method, establishes a new standard for distance metric learning research while providing immediate practical value for practitioners working with challenging datasets.

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