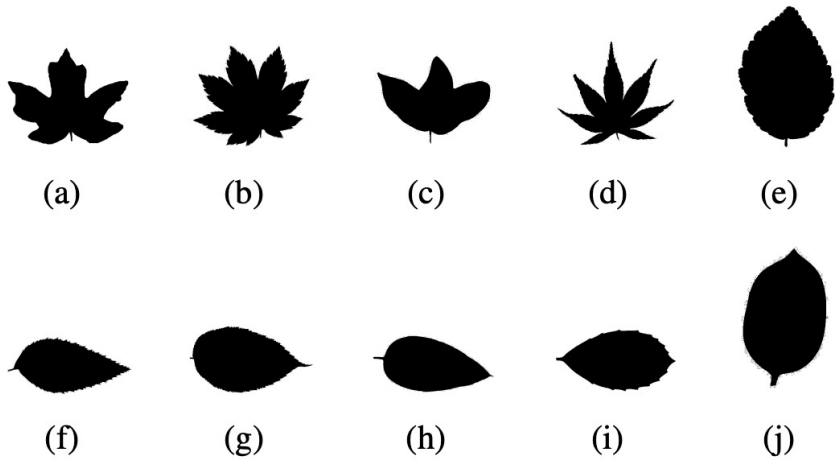
Comparing Multivariate Embedding Methods for Plant Species Identification

March 26, 2025

Introduction



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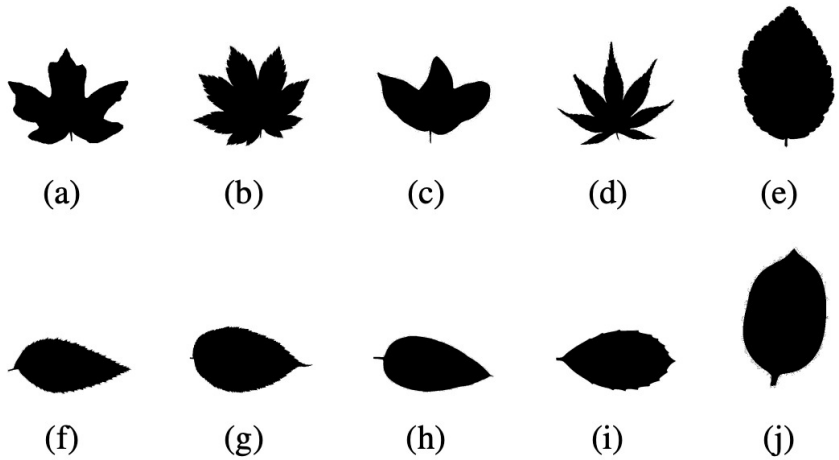

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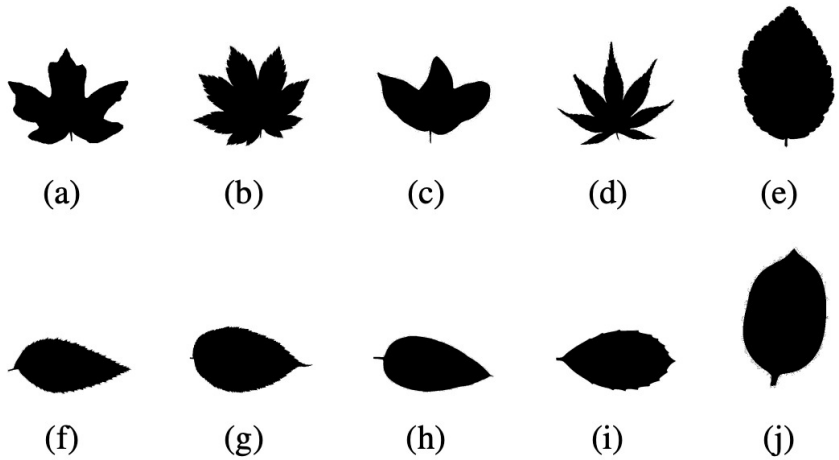

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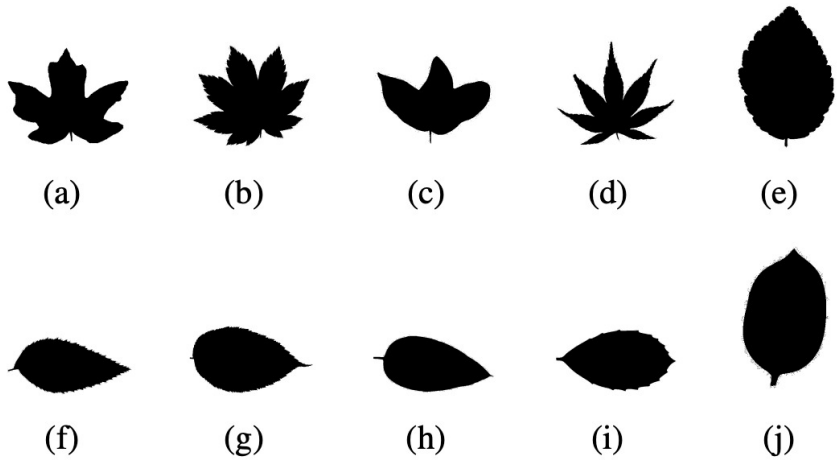

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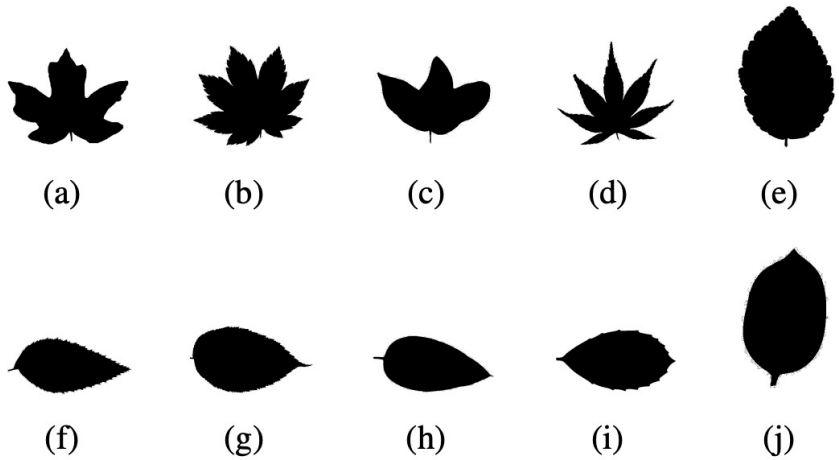

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- 192 features: 64 each of shape, margin and pattern
- Extension- apply dimension reduction before clustering:
  1. Principal Component Analysis (PCA)
  2. Isometric Mapping (Isomap)
  3. Locally Linear Embedding (LLE)

Principal Component Analysis

Steps:

1. Calculate the Principal Components (PC's) from the correlation matrix
2. Determine the number of PC's to keep using a Scree plot

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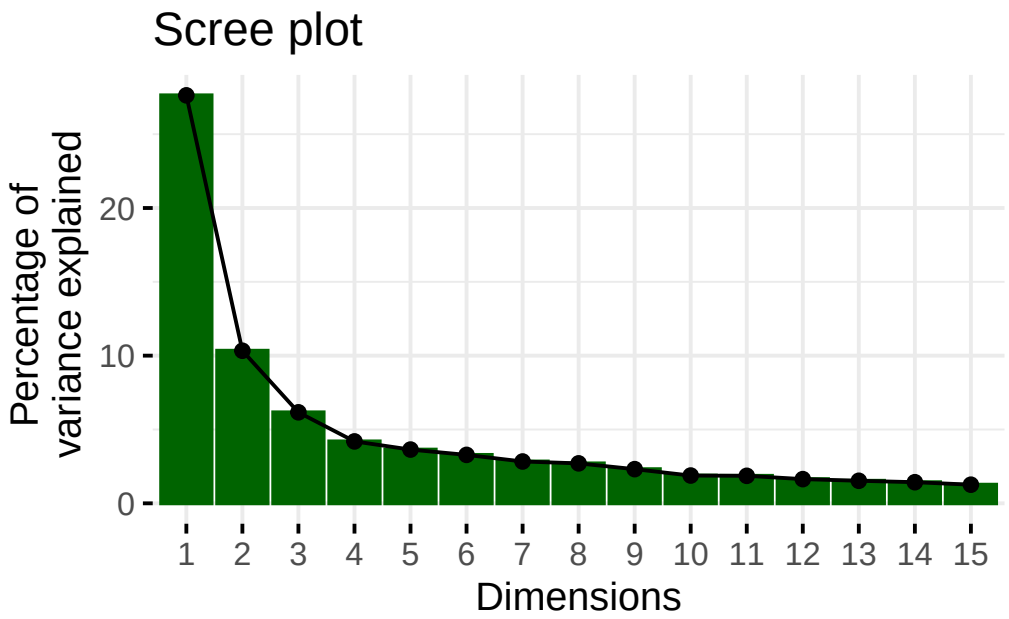

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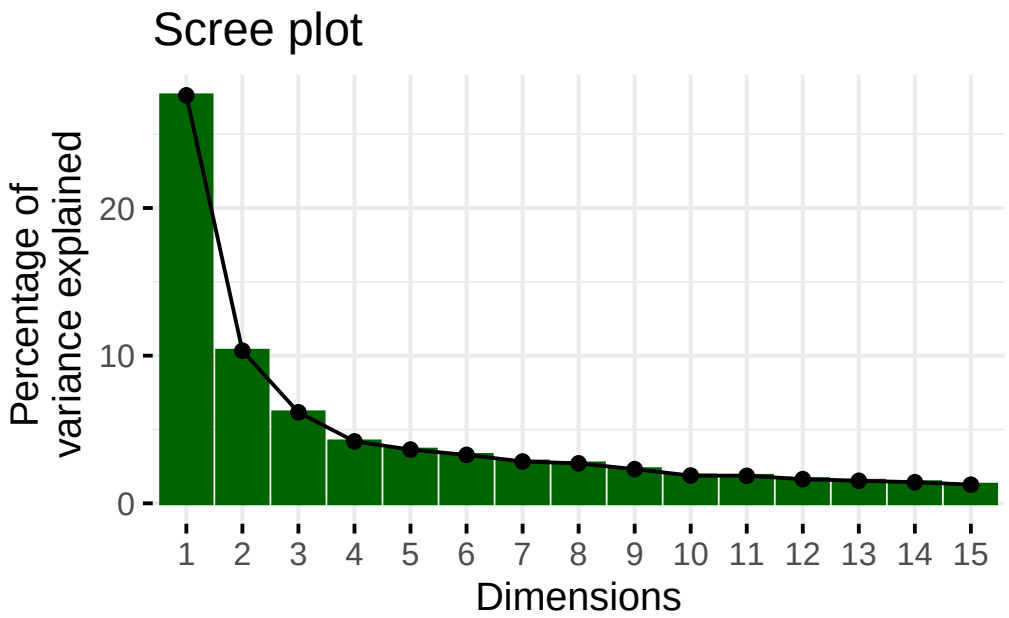

- Lower dimensional embedding to be used: {4 PCs}, {10 PCs}, {30 PCs}

Isometric Mapping

Steps:

1. Construct neighborhood graph
2. (Find k_{min})
3. Calculate geodesic distances
4. Apply MDS
5. Calculate residual variance

Isometric Mapping

Residual variance

$$\text{Residual Variance} = 1 - R^2 = 1 - \text{cor}^2(D_G, D_Y) \quad (1)$$

1. D_G: matrix of geodesic distances between all pairs of observations in $\mathbb{R}^D$
2. D_Y: matrix of Euclidean distances between all pairs of observations in $\mathbb{R}^d$

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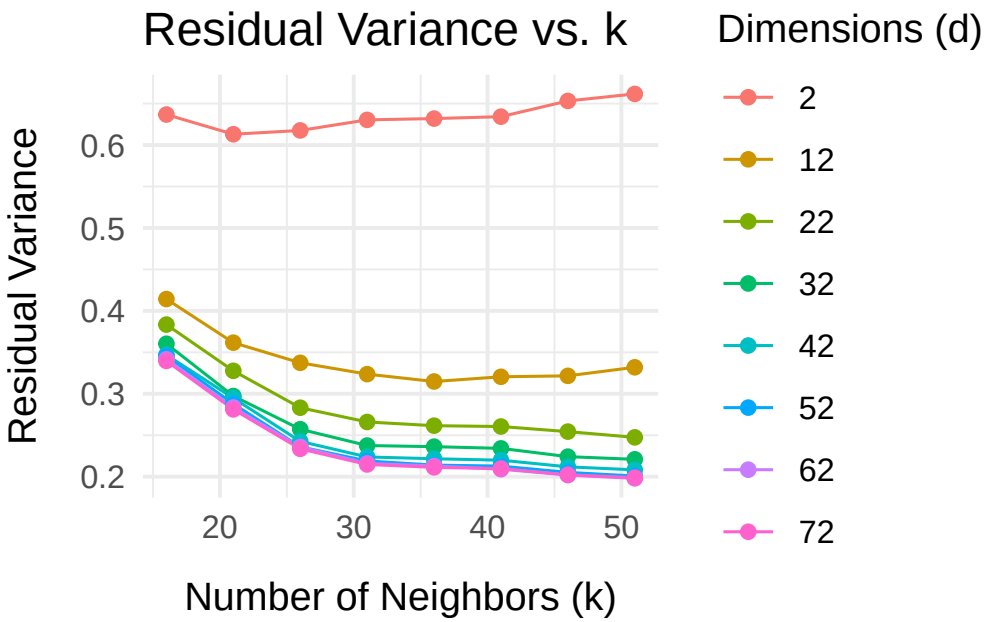

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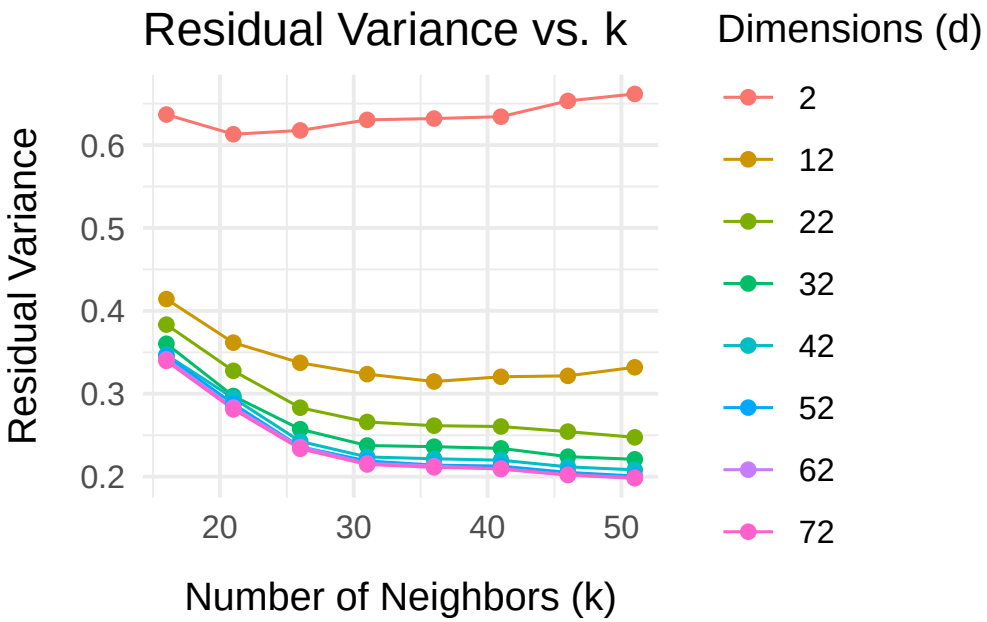

- Lower dimensional embedding to be used: $\{d = 22,\ k = 16\}$, $\{d = 22,\ k = 21\}$, $\{d = 22,\ k = 26\}$

Locally Linear Embedding

Steps:

1. Find the K-NN of each observation

Locally Linear Embedding

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2. Calculate w_{ij}

Locally Linear Embedding

w_{ij} calculation

$$\mathbf{x}_i \approx \sum_{j \in N(i)} w_{ij} \mathbf{x}_j \quad \forall\ i = 1, \ldots, N \tag{2}$$

subject to

$$\sum_j w_{ij} = 1 \tag{3}$$

$$w_{ij} = 0 \quad \forall\ j \notin N(i) \tag{4}$$

Locally Linear Embedding

Steps:

1. Find the K-NN of each observation
2. Calculate w_{ij}
3. Calculate lower dimensional embedding $\mathbf{Y}$

Locally Linear Embedding

Minimize the Reconstruction Error

$$\Phi(\mathbf{Y}) = \sum_{i=1}^{N} \left\| \mathbf{y}_i - \sum_{j} w_{ij} \mathbf{y}_j \right\|^2 \tag{5}$$

where

$$\mathbf{Y} \in \mathbb{R}^{n \times d} \tag{6}$$

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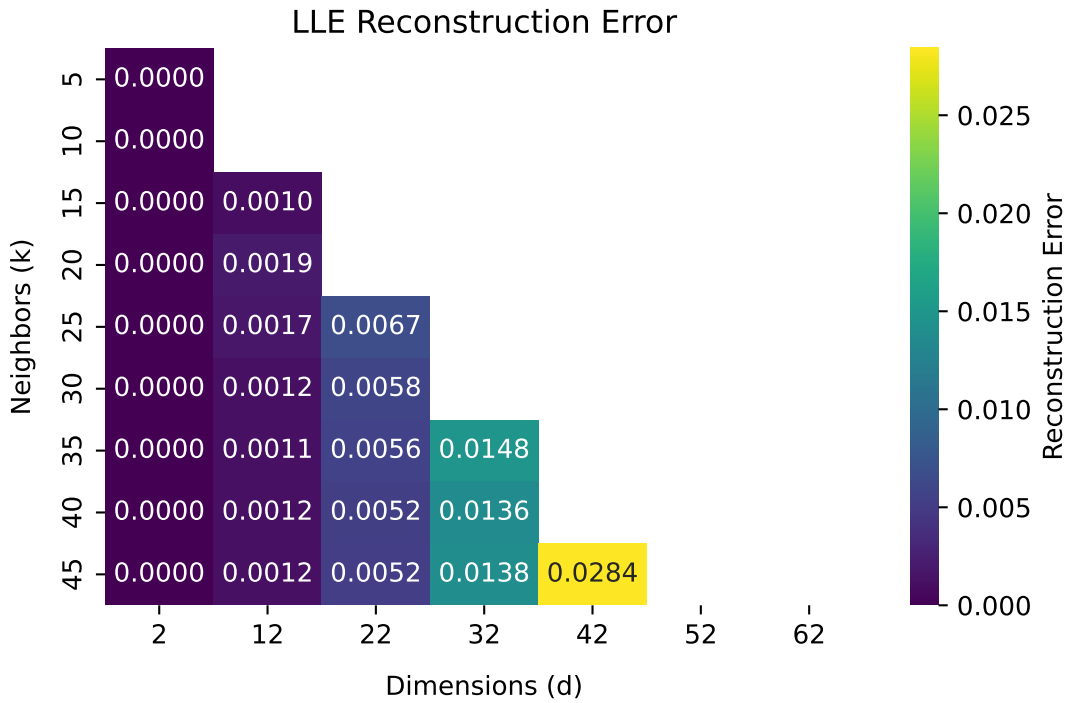

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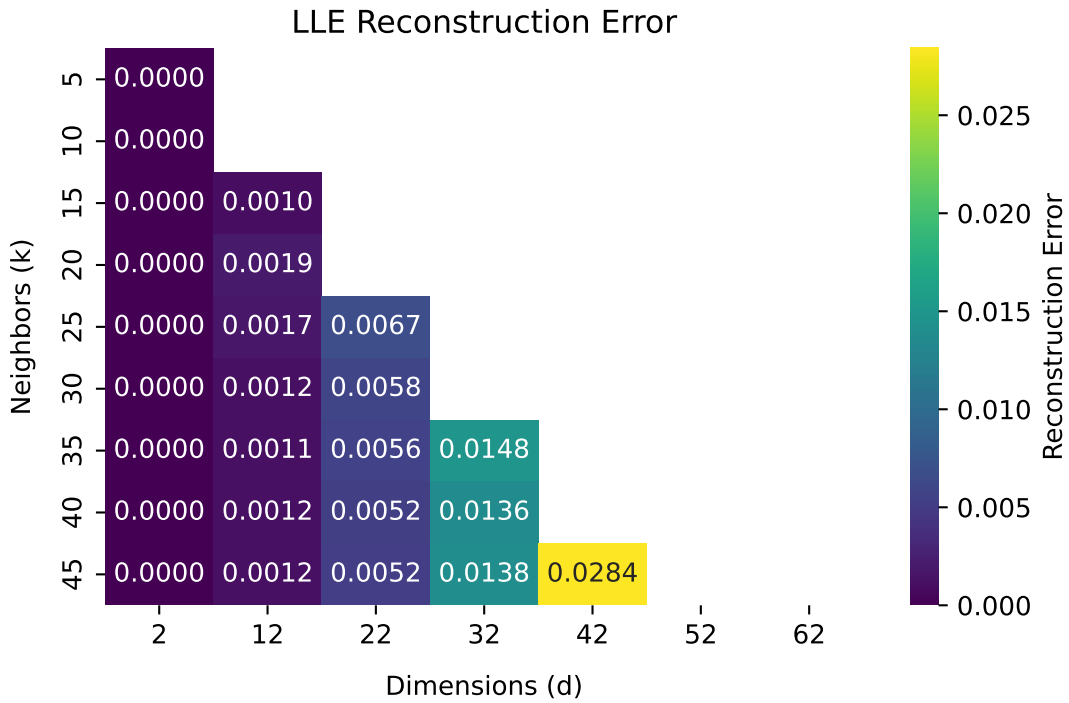

- Lower dimensional embedding to be used: $\{d = 2,\ k = 15\}$, $\{d = 12,\ k = 15\}$, $\{d = 22,\ k = 25\}$, $\{d = 32,\ k = 35\}$, $\{d = 42,\ k = 45\}$

What's left?

- Apply a clustering algorithm
  1. K-Means
  2. Kernel K-Means
- Determine if dimension reduction improved the results

Comments and discussion

Questions?

References

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