Machine Intelligence 2

4.4 Locally Linear Embedding

Prof. Dr. Klaus Obermayer

Fachgebiet Neuronale Informationsverarbeitung (NI)

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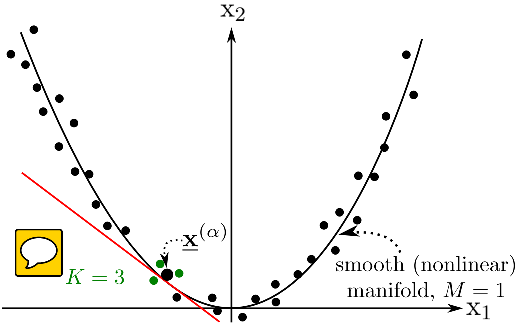
Locally Linear Embedding

Project data into the tangential (linear) space of the data manifold



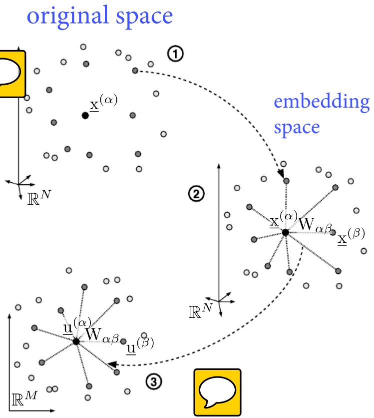
- data points $\underline{\mathbf{x}}^{(\alpha)} \in \mathbb{R}^N$
- embedded data points $\underline{\mathbf{u}}^{(\alpha)} \in \mathbb{R}^M, \quad M < N$

Locally Linear Embedding

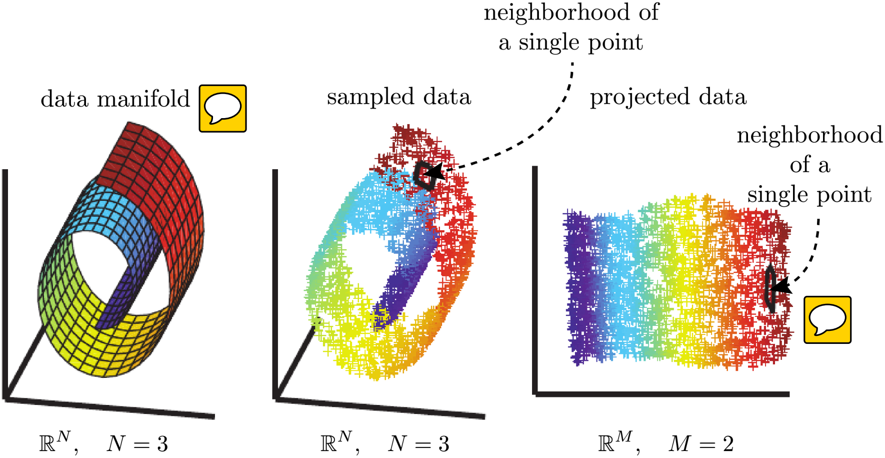
Project data into the tangential (linear) space of the data manifold

For each data point $\underline{\mathbf{x}}^{(\alpha)}$

- find the K nearest neighbors
- calculate reconstruction weights $\underline{\mathbf{W}}$
  s.t. $\underline{\mathbf{x}}^{(\alpha)} \approx \sum_{\beta \in \mathrm{KNN}(\underline{\mathbf{x}}^{(\alpha)})} \mathrm{W}_{\alpha\beta} \cdot \underline{\mathbf{x}}^{(\beta)}$
- obtain embedding $\underline{\mathbf{u}}^{(\alpha)} \in \mathbb{R}^M$
  s.t. $\underline{\mathbf{u}}^{(\alpha)} \approx \sum_{\beta \in \mathrm{KNN}(\underline{\mathbf{x}}^{(\alpha)})} \mathrm{W}_{\alpha\beta} \cdot \underline{\mathbf{u}}^{(\beta)}$



Locally Linear Embedding



Source: Science; Roweis, Saul 2000, modified

Step 1: find K nearest neighbors

choice: Euclidean distance

$$
\begin{aligned}
\beta_1^{(\alpha)} &= \arg\min_{\beta} \left| \underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{x}}^{(\beta)} \right| \\
\beta_2^{(\alpha)} &= \arg\min_{\beta \neq \beta_1^{(\alpha)}} \left| \underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{x}}^{(\beta)} \right| \\
&\vdots \\
\beta_K^{(\alpha)} &= \arg\min_{\substack{\beta \neq \beta_k^{(\alpha)}, \\ k=1,\ldots,K-1}} \left| \underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{x}}^{(\beta)} \right| \\
\mathrm{KNN}(\underline{\mathbf{x}}^{(\alpha)}) &= \left\{ \beta_1^{(\alpha)}, \beta_2^{(\alpha)}, \ldots, \beta_K^{(\alpha)} \right\} \quad \text{(not necessarily unique)}
\end{aligned}
$$

linear data structure (e.g. data matrix): $\mathcal{O}(Np^2)$
k-d tree (balanced search tree): $\mathcal{O}(Np \log p)$

oneNote

Step 2: calculate reconstruction weights

minimize cost function:

$$E(\underline{\mathbf{W}}) = \sum_{\alpha=1}^{p} \underbrace{\left| \underline{\mathbf{x}}^{(\alpha)} - \sum_{\beta=1}^{p} \mathrm{W}_{\alpha\beta} \underline{\mathbf{x}}^{(\beta)} \right|^2}_{\substack{\text{reconstruct } \underline{\mathbf{x}}^{(\alpha)} \text{ by its} \\ K \text{ nearest neighbors only}}} \stackrel{!}{=} \min \quad \text{s.t.} \quad \begin{array}{l} \mathrm{W}_{\alpha\beta} = 0 \text{ if } \beta \notin \mathrm{KNN}(\underline{\mathbf{x}}^{(\alpha)}), \\ \sum_{\beta=1}^{p} \mathrm{W}_{\alpha\beta} = 1 \end{array}$$

weight matrix $\underline{\mathbf{W}}$:

- sparse: (up to) K nonzero elements per row
- not symmetric: nearest neighbors of a data point can have closer neighbors

Step 2: calculate reconstruction weights

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optimal weights are invariant to:

- rotation $\underline{\mathbf{R}}$: $\quad E\left[\underline{\mathbf{R}} \cdot \underline{\mathbf{x}}^{(1)}, \ldots, \underline{\mathbf{R}} \cdot \underline{\mathbf{x}}^{(p)}\right] \overset{\text{orthog. } \underline{\mathbf{R}}}{=} E\left[\underline{\mathbf{x}}^{(1)}, \ldots, \underline{\mathbf{x}}^{(p)}\right]$
- scaling $\gamma > 0$: $\quad E\left[\gamma \underline{\mathbf{x}}^{(1)}, \ldots, \gamma \underline{\mathbf{x}}^{(p)}\right] = \gamma^2 E\left[\underline{\mathbf{x}}^{(1)}, \ldots, \underline{\mathbf{x}}^{(p)}\right]$
- translation $\Delta \underline{\mathbf{x}}$: $\quad E\left[\underline{\mathbf{x}}^{(1)} + \Delta \underline{\mathbf{x}}, \ldots, \underline{\mathbf{x}}^{(p)} + \Delta \underline{\mathbf{x}}\right] \overset{\sum_\beta \mathrm{W}_{\alpha\beta} = 1}{=} E\left[\underline{\mathbf{x}}^{(1)}, \ldots, \underline{\mathbf{x}}^{(p)}\right]$

Step 2: calculate reconstruction weights

oneNote

minimize cost function:

$$E(\underline{\mathbf{W}}) = \sum_{\alpha=1}^{p} \underbrace{\left| \underline{\mathbf{x}}^{(\alpha)} - \sum_{\beta=1}^{p} \mathrm{W}_{\alpha\beta} \underline{\mathbf{x}}^{(\beta)} \right|^2}_{\substack{\text{reconstruct } \underline{\mathbf{x}}^{(\alpha)} \text{ by its} \\ K \text{ nearest neighbors only}}} \stackrel{!}{=} \min \quad \text{s.t.} \quad \mathrm{W}_{\alpha\beta} = 0 \text{ if } \beta \notin \mathrm{KNN}(\underline{\mathbf{x}}^{(\alpha)}), \quad \sum_{\beta=1}^{p} \mathrm{W}_{\alpha\beta} = 1$$

for each data point $\underline{\mathbf{x}}^{(\alpha)}$:

- local "covariance" matrix (symmetric & positive semidefinite) $\underline{\mathbf{C}}^{(\alpha)} \in \mathbb{R}^{K,K}$:

$$\mathrm{C}_{jk} = \left(\underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{x}}^{(\beta_j^{(\alpha)})}\right)^T \left(\underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{x}}^{(\beta_k^{(\alpha)})}\right)$$

- solve linear system $\underline{\mathbf{C}}^{(\alpha)} \underline{\widetilde{\mathbf{w}}}^{(\alpha)} = (1, \ldots, 1)^T$
- rescale weights: $\mathrm{W}_{\alpha\beta_j^{(\alpha)}} = \widetilde{\mathrm{w}}_j^{(\alpha)} / \sum_{k=1}^{K} \widetilde{\mathrm{w}}_k^{(\alpha)}$ to fulfill constraint

$\Rightarrow$ $\underline{\mathbf{W}}$ contains the optimal weights with $\mathrm{W}_{\alpha\beta} = 0$ for $\beta \notin \mathrm{KNN}(\underline{\mathbf{x}}^{(\alpha)})$

$\Rightarrow$ p dense K-dim. linear systems have to be solved: $\mathcal{O}(pK^3)$

Step 3: obtain embedding coordinates

For any M-dimensional manifold there exist linear mappings of each local "patch" onto M-dimensional coordinates in a linear space

- linear mapping: rotation, scaling, translation
- weights $\underline{\mathbf{W}}$ can be used to optimally reconstruct the data points in the lower-dimensional embedding space

idea:

- cut N-d manifold into small patches
- "glue" them together in M-d using only rotation, scaling, translation for each patch

Step 3: obtain embedding coordinates

given $M \ll N$ and $\underline{\mathbf{W}}$: find optimal coordinates $\underbrace{\underline{\mathbf{u}}^{(1)}, \ldots, \underline{\mathbf{u}}^{(p)}}_{= \underline{\mathbf{U}} \in \mathbb{R}^{M,p}} \in \mathbb{R}^M$

cost function:

$$F(\underline{\mathbf{U}}) = \sum_{\alpha=1}^{p} \left| \underline{\mathbf{u}}^{(\alpha)} - \sum_{\beta=1}^{p} \mathrm{W}_{\alpha\beta} \underline{\mathbf{u}}^{(\beta)} \right|^2$$

equivalent quadratic form:

$$F(\underline{\mathbf{U}}) = \sum_{\alpha,\beta=1}^{p} g_{\alpha\beta} (\underline{\mathbf{u}}^{(\alpha)})^T \underline{\mathbf{u}}^{(\beta)}$$

where $g_{\alpha\beta} =$

see blackboard

$$= \delta_{\alpha\beta} - \mathrm{W}_{\alpha\beta} - \mathrm{W}_{\beta\alpha} + \sum_{\gamma=1}^{p} \mathrm{W}_{\gamma\alpha} \mathrm{W}_{\gamma\beta}$$

$\underline{\mathbf{G}} = \{ g_{\alpha\beta} \} \in \mathbb{R}^{p,p}$ is symmetric and positive semidefinite

Step 3: obtain embedding coordinates

minimize cost function:

$$F(\underline{\mathbf{U}}) = \sum_{\alpha,\beta=1}^{p} g_{\alpha\beta} (\underline{\mathbf{u}}^{(\alpha)})^T \underline{\mathbf{u}}^{(\beta)}$$

s.t. $\sum_{\alpha=1}^{p} \underline{\mathbf{u}}^{(\alpha)} = 0,$ (remove translation freedom)

$\frac{1}{p} \sum_{\alpha=1}^{p} \underline{\mathbf{u}}^{(\alpha)} (\underline{\mathbf{u}}^{(\alpha)})^T = \underline{\mathbf{I}}$ (prevent trivial solutions e.g., $\underline{\mathbf{u}}^{(\alpha)} = \underline{\mathbf{0}}$)

- $\leadsto$ w.l.o.g. as $F(\underline{\mathbf{U}})$ invariant to rotation, scaling, translation
- $\leadsto$ implies that reconstruction errors for different coordinates are measured on the same scale

Step 3: obtain embedding coordinates

solution:

compute the $M + 1$ eigenvectors of $\underline{\mathbf{G}}$ with the lowest eigenvalues but discard the eigenvector $\underline{\mathbf{e}}_p = \frac{1}{p}(1, \ldots, 1)^T$ with eigenvalue 0 (corresponding to translation)

$$\underline{\mathbf{U}} = \begin{pmatrix} \underline{\mathbf{e}}_{p-M}^T \\ \vdots \\ \underline{\mathbf{e}}_{p-1}^T \end{pmatrix} = \left(\underline{\mathbf{u}}^{(1)}, \ldots, \underline{\mathbf{u}}^{(p)}\right) \quad \text{(solution satisfies both constraints)}$$

implementation:

- store $\underline{\mathbf{W}}$ in sparse matrix format (at most $K \cdot p$ non-zero elements) and calculate $\underline{\mathbf{G}} = \left(\underline{\mathbf{I}} - \underline{\mathbf{W}}^T\right)\left(\underline{\mathbf{I}} - \underline{\mathbf{W}}\right) \in \mathbb{R}^{p,p}$
- use sparse eigenvalue solvers (eigsh)

$$\underline{\mathbf{v}} \mapsto \underline{\mathbf{G}} \cdot \underline{\mathbf{v}} = \left(\underline{\mathbf{I}} - \underline{\mathbf{W}}^T\right)\left[\left(\underline{\mathbf{I}} - \underline{\mathbf{W}}\right)\underline{\mathbf{v}}\right]$$

Summary of the LLE algorithm

parameters: K, M

1. find K nearest neighbors $\mathrm{KNN}(\underline{\mathbf{x}}^{(\alpha)}) = \left\{\beta_1^{(\alpha)}, \dots, \beta_K^{(\alpha)}\right\} \; \forall \alpha = 1, \dots, p$
2. calculate (locally invariant) reconstruction weights $\underline{\mathbf{W}}$:

$$\underline{\mathbf{C}}^{(\alpha)} \underline{\widetilde{\mathbf{w}}}^{(\alpha)} = (1, \dots, 1)^T, \quad \forall \alpha = 1, \dots, p$$

$$\mathrm{W}_{\alpha \beta_j^{(\alpha)}} = \frac{\widetilde{\mathrm{w}}_j^{(\alpha)}}{\sum_{k=1}^{K} \widetilde{\mathrm{w}}_k^{(\alpha)}}$$

3. calculate the embedding coordinates $\underline{\mathbf{U}}$:

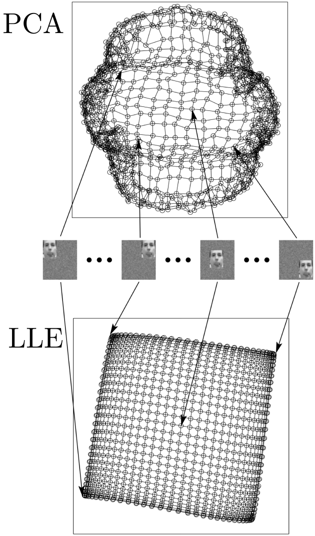
   compute the $M+1$ eigenvectors $\left(\underline{\mathbf{e}}_p, \dots, \underline{\mathbf{e}}_{p-M}\right)$ of $\underline{\mathbf{G}}$
   with the smallest eigenvalues

$$g_{\alpha\beta} = \delta_{\alpha\beta} - \mathrm{W}_{\alpha\beta} - \mathrm{W}_{\beta\alpha} + \sum_{\gamma=1}^{p} \mathrm{W}_{\gamma\alpha} \mathrm{W}_{\gamma\beta}$$

$$\underline{\mathbf{G}} \cdot \underline{\mathbf{e}}_j = \lambda_j \underline{\mathbf{e}}_j \qquad \underline{\mathbf{U}} = \begin{pmatrix} \underline{\mathbf{e}}_{p-M}^T \\ \vdots \\ \underline{\mathbf{e}}_{p-1}^T \end{pmatrix} = \left(\underline{\mathbf{u}}^{(1)}, \dots, \underline{\mathbf{u}}^{(p)}\right)$$

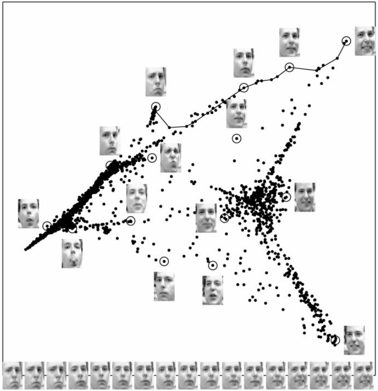
Example 1

- Images of a single face translated across a two-dimensional background of noise
- PCA fails to preserve the neighborhood structure of nearby images
- LLE maps the images with corner faces to the corners of its two dimensional embedding



Source: An Introduction to Locally Linear Embedding; Saul, Roweis 2001

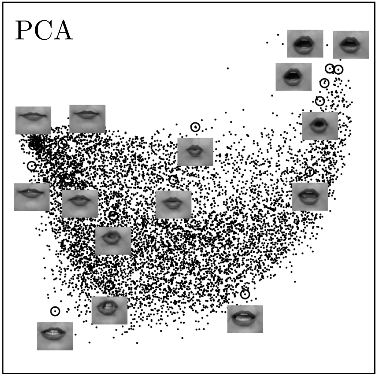
Example 2

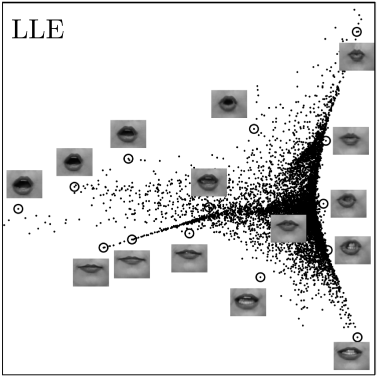


Source: Science; Roweis, Saul 2000

- Images of faces mapped into an embedding space with $M = 2$.
- Bottom: Images corresponding to points along the solid line shown on the top-right.

Example 3





Source: An Introduction to Locally Linear Embedding; Saul, Roweis 2001

- Images of lips mapped into an embedding space with $M = 2$.
- Differences between the two embeddings indicate the presence of nonlinear structure in the data.

Remarks

- efficient & robust algorithm
- parameters: number K of neighbors, embedding dimension M
- convex optimization problem, standard (sparse) linear algebra methods suffice
- for $K > N$ regularization is required (singular covariance matrix $\underline{\mathbf{C}}^{(\alpha)}$)

$$\underline{\mathbf{C}}^{(\alpha)} \leftarrow \underline{\mathbf{C}}^{(\alpha)} + \varepsilon \underline{\mathbf{I}}$$

- extension for pairwise data available via non-Euclidean distances $d_{\alpha\alpha'}$ in $\underline{\mathbf{C}}^{(\alpha)}$
- alternative methods available (e.g. Laplacian eigenmaps, t-stochastic neighbor embedding, isomap, multi-dimensional scaling, Kernel PCA)