# Non-Linear Dimensionality Reduction

Presentation by Daniel Steinberg

CS3750, Fall 2011

Some Slides are New but Most are From or Have been Adapted From:
Fall 2011 Slides by Md. Abedul Haque,
Fall 2011 Slides by Saeed Amizadeh,
And Slides by Iyad Batal

### **Outline**

- Linear Dimensionality Reduction
  - PCA
  - MDS
- Non-Linear Dimensionality Reduction
  - Laplacian Eigenmaps
  - Locally Linear Embedding
  - Isomap

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### **Dimensionality Reduction**

- Linear Dimensionality Reduction Methods
  - PCA
    - Finds a low-dimensional embedding of the data points that maximizes the variance of the projected data
  - Classical MDS
    - Finds an embedding that preserves the inter-point distances.
    - Equivalent to PCA when those distances are Euclidean.

### Multi-Dimensional Scaling (MDS)

- Multi-Dimensional Scaling [Cox and Cox, 1994] .
- MDS give points in a low dimensional space such that the Euclidean distances between them best approximate the original distance matrix.
   Given distance matrix

(I is number of observations)

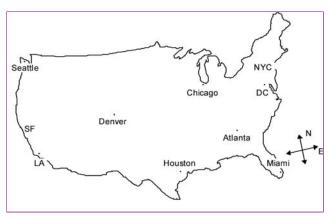
$$\Delta := \begin{pmatrix} \delta_{1,1} & \delta_{1,2} & \cdots & \delta_{1,I} \\ \delta_{2,1} & \delta_{2,2} & \cdots & \delta_{2,I} \\ \vdots & \vdots & & \vdots \\ \delta_{I,1} & \delta_{I,2} & \cdots & \delta_{I,I} \end{pmatrix}.$$

Map input point pairs  $(x_i, x_j)$  to  $(z_i, z_j)$  such that  $||z_i - z_j|| \approx \delta_{i,j}$ 

- Classical MDS: the norm || . || is the Euclidean distance.
- $\min_{z_1,...z_I} \sum_{i < j} (||z_i z_j|| \delta_{i,j})^2$ 
  - From Wikipedia: A solution may then be found by numerical optimization techniques. For some particularly chosen cost functions, minimizers can be stated analytically in terms of matrix eigendecompositions.
    - "Citation Needed" on Wikipedia
    - This is the same approach of how Laplacian Eigenmap is solved

### MDS example

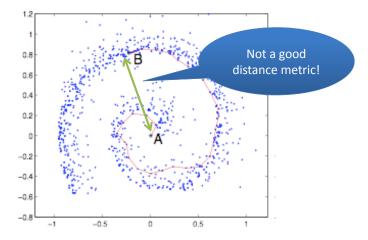
 Given pairwise distances between different cities in 3D (Δ matrix), plot the cities on a 2D plane (recover location)



### PCA and MDS relation

- Preserve Euclidean distances = retaining the maximum variance.
- Classical MDS is equivalent to PCA when the distances in the input space are the <u>Euclidean</u> distance.
- If we have only a distance matrix (we don't know the points in the original space), we cannot perform PCA
- Both PCA and MDS are invariant to space rotation

### Underestimation of distance



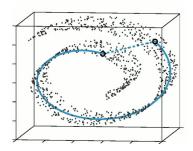
- For local distances, Euclidean distance may be sufficient
- For global distances, Euclidean distance may underestimate
  - In example above, desired distance between A and B is along the red line. Euclidean distance is an underestimate, as can be seen by the green arrow.

### Outline

- Linear Dimensionality Reduction
  - -PCA
  - MDS
- Non-Linear Dimensionality Reduction
  - Laplacian Eigenmaps
  - Locally Linear Embedding
  - Isomap

### Non-Linear Dimensionality Reduction

- A special class of problem
  - Low dimensional data lying on a manifold in a higher dimensional space

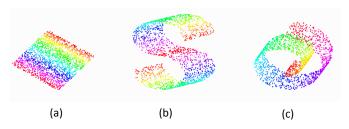


### Manifolds



- Three examples of manifolds
- All three are two-dimensional manifolds embedded in 3 dimensions
  - Linear, "S"-shape, "Swiss roll"
- For all three, we would like to recover:
  - That the data is only two-dimensional
  - "Consistent" locations for the data in 2D

### Manifolds

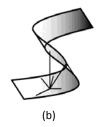


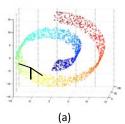
- PCA: works for (a)
- Doesn't do much good for (b) or (c)
  - Linear subspace doesn't explain it well
- What do we mean by "consistent locations"?
  - Preserve local relationships and structure
  - One possibility: preserve distances

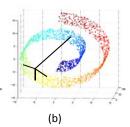
### Preserving Local/Global Relationships

- MDS produces a linear embedding
  - Preserved all pairwise distances









- Nonlinear manifold:
  - local distances (a) make sense
  - but, global distances (b) don't respect the geometry

### **Dimensionality Reduction**

- Methods that preserve local structure
  - Laplacian Eigenmaps
  - Locally Linear Embedding (LLE)
  - Isomap

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### **Laplacian Matrix Components**

- Given Graph G
- Let e<sub>ij</sub> = edge weight from node i to node j
  Weight Matrix W (e.g., Heat Kernel)

$$w_{ij} = \begin{cases} e_{ij} & \text{if i is adjacent to j} \\ 0 & \text{otherwise} \end{cases}$$

- Matrix D
  - Diagonal Matrix with diagonal elements containing column sums of W. Since W is symmetric, using row sums is equivalent.
  - Often Referred to as a Degree Matrix when all edge weights are 1 (that is, when W is the adjacency matrix)

$$d_{ij} = \begin{cases} \sum_{j} w_{ij} & \text{if i = j (diagonal element)} \\ 0 & \text{otherwise} \end{cases}$$

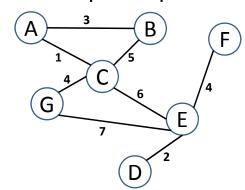
### Laplacian Matrix

- Laplacian Matrix L = D − W
- L is positive semidefinite (PSD)
  - We will show why later
  - We will use this property for optimization

A symmetric square Matrix  $\mathbf{A} \in \mathbb{R}^{n \times n}$  is positive semidefinite if for all  $\mathbf{x} \in \mathbb{R}^n$ ,  $\mathbf{x}^\mathsf{T} \mathbf{A} \mathbf{x} \ge 0$ .

 $\mathbf{x}^{\mathsf{T}}\mathbf{A}\mathbf{x}$  is called a *quadratic form*.

### Example: Laplacian Matrix of a Graph



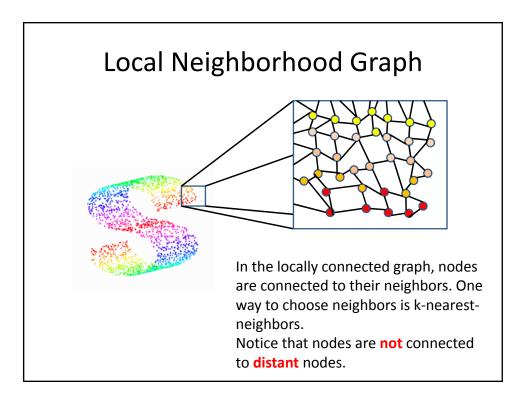
Note: Node A corresponds to row 1 and column 1, Node B to row 2 and column 2, ..., Node G to row 7 and column 7

$$\mathbf{W} = \begin{bmatrix} 0 & 3 & 1 & 0 & 0 & 0 & 0 \\ 3 & 0 & 5 & 0 & 0 & 0 & 0 \\ 1 & 5 & 0 & 0 & 6 & 0 & 4 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 6 & 2 & 0 & 4 & 7 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 & 7 & 0 & 0 \end{bmatrix}$$

$$\mathbf{D} = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 16 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 19 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 11 \end{bmatrix} \quad \mathbf{L} = \mathbf{D} - \mathbf{W} = \begin{bmatrix} 4 & -3 & -1 & 0 & 0 & 0 & 0 \\ -3 & 8 & -5 & 0 & 0 & 0 & 0 & 0 \\ -1 & -5 & 16 & 0 & -6 & 0 & -4 \\ 0 & 0 & 0 & 2 & -2 & 0 & 0 \\ 0 & 0 & -6 & -2 & 19 & -4 & -7 \\ 0 & 0 & 0 & 0 & -4 & 4 & 0 \\ 0 & 0 & -4 & 0 & -7 & 0 & 11 \end{bmatrix}$$

### Laplacian Eigenmaps Overview

- We have n data points in d dimensions
- We want to project the data onto a lower dimension k
- In lower dimension, relative distances between points should preserve relative distances (along the manifold) from the higher dimensional space.
- Algorithm Overview
  - Form a graph G where nodes correspond to data points and are connected to local nodes
  - Weight the edges of graph G according to local distances between nodes [data points]
  - Compute matrices W, D, and Laplacian matrix L of graph G
  - Compute Eigenvalues and Eigenvectors of (D<sup>-1</sup>L)
  - Use k eigenvectors corresponding to smallest non-zero eigenvalues, to project data onto k dimensions.



### Laplacian Eigenmaps Algorithm

- Step 1: Construct the graph
  - Construct the adjacency graph G by connecting neighboring nodes (i,j)
- Neighbors selection
  - $\epsilon$ -neighborhoods  $\|x_i x_j\|^2 < \epsilon$ 
    - Advantages
      - Geometrically motivated
      - Relationships are symmetric
    - Disadvantages
      - Can lead to Disconnected graphs
      - − Difficult to choose €
  - n nearest neighbors
    - Advantages
      - Easier to choose
      - No disconnected graphs
    - Disadvantages
      - Less geometrically intuitive (asymmetric relationships)

### Laplacian Eigenmaps Algorithm

- Step 2: Choose the weights
  - Simple-minded
    - 1 if connected
    - 0 otherwise
  - Heat Kernel
    - $\mathbf{W}_{ij} = e^{\frac{-\left\|x_i x_j\right\|^2}{t}}$  if connected
    - 0 otherwise
  - Heat kernel with  $t=\infty$  is equivalent to the  $\emph{simple-minded}$  approach

### Laplacian Eigenmaps Algorithm

- Step 3: Eigenmaps
  - Construct Laplacian matrix
    - Construct diagonal weight matrix D from weight matrix.  $D_{ii} = \sum_{i} W_{ii}$
    - Construct Laplacian matrix L = D W
      - W, and thus L, will be sparse. Nodes [data points] are only connected to nearby [similar] nodes.
  - Laplacian is a symmetric, positive semi-definite matrix
  - Compute eigenvalues and eigenvectors of the generalized eigenvector problem:

$$Lf = \lambda Df$$

Alternative (but equivalent) formulation:
 Find eigenvalues and eigenvectors of matrix (D<sup>-1</sup>L)

$$(D^{-1}L)\mathbf{f} = \lambda \mathbf{f}$$

### Laplacian Eigenmaps Algorithm

• Step 3: Eigenmaps

$$Lf = \lambda Df$$

— Let,  $f_0$ ,  $f_1$ , ...,  $f_{k-1}$  be the solutions ordered according to increasing eigenvalues

$$\begin{split} \mathbf{L}\mathbf{f}_0 &= \lambda_0 \mathbf{D}\mathbf{f}_0 \\ \mathbf{L}\mathbf{f}_1 &= \lambda_1 \mathbf{D}\mathbf{f}_1 \\ \dots \\ \mathbf{L}\mathbf{f}_{k-1} &= \lambda_{k-1} \mathbf{D}\mathbf{f}_{k-1} \\ \mathbf{0} &= \lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_{k-1} \end{split}$$

— We leave out eigenvector  $\mathbf{f}_0$ . Take the next m eigenvectors to construct m-dimensional embedding  $(\mathbf{f}_1(i), ..., \mathbf{f}_m(i))$ 

### Laplacian Eigenmaps Motivation

- Consider the problem of mapping weighted graph G into a line so that the connected nodes stay as close as possible
- Let  $\mathbf{y} = (y_1, y_2, ..., y_n)^T$  be such a map
- A "reasonable criterion" for a good map is to minimize  $\sum_{ij} (y_i y_j)^2 W_{ij}$
- - The constraint removes arbitrary scaling factor
- From equation \* above, L is positive semidefinite since  $(y_i-y_j)^2 \ge 0$  and  $W_{ij} \ge 0$
- Since L is positive semidefininte, the solution to our minimization problem is the generalized eigenvalue solution
  - Ly = λDy
- 1 is an eigenvector corresponding to eigenvalue 0.
- To eliminate this trivial solution, add constraint  $\mathbf{y}^T \mathbf{D} \mathbf{1} = 0$

# Derive $\sum_{ij} (y_i - y_j)^2 W_{ij} = 2y^T Ly$ (from previous slide)

$$\sum_{i,j} (y_i - y_j)^2 \mathbf{W}_{i,j} = \sum_{i,j} (y_i - y_j) (y_i - y_j) \mathbf{W}_{i,j}$$

$$= \sum_{i,j} (y_i^2 - 2y_i y_j + y_j^2) \mathbf{W}_{i,j}$$

$$= \sum_{i,j} y_i^2 \mathbf{W}_{i,j} - \sum_{i,j} 2y_i y_j \mathbf{W}_{i,j} + \sum_{i,j} y_j^2 \mathbf{W}_{i,j}$$

$$= \sum_{i} y_i^2 \sum_{j} \mathbf{W}_{i,j} - 2 \sum_{i,j} y_i y_j \mathbf{W}_{i,j} + \sum_{j} y_j^2 \sum_{i} \mathbf{W}_{i,j}$$

$$= \sum_{i} y_i^2 \sum_{j} \mathbf{W}_{i,j} + \sum_{j} y_j^2 \sum_{i} \mathbf{W}_{i,j} - 2 \sum_{i,j} y_i y_j \mathbf{W}_{i,j}$$

$$= \sum_{i} y_i^2 \mathbf{D}_{i,i} + \sum_{j} y_j^2 \mathbf{D}_{j,j} - 2 \sum_{i,j} y_i y_j \mathbf{W}_{i,j}$$

$$= 2 \sum_{i} y_i^2 \mathbf{D}_{i,i} - 2 \sum_{i,j} y_i y_j \mathbf{W}_{i,j}$$

$$= 2 \mathbf{y}^T \mathbf{D} \mathbf{y} - 2 \mathbf{y}^T \mathbf{W} \mathbf{y}$$

$$= 2 \mathbf{y}^T (\mathbf{D} - \mathbf{W}) \mathbf{y}$$

$$= 2 \mathbf{y}^T \mathbf{L} \mathbf{y}$$

### Notes:

Matrix  $\mathbf{A} \in \mathbb{R}^{n \times n}$  and  $\mathbf{x} \in \mathbb{R}^n$ ,  $\mathbf{x}^\mathsf{T} \mathbf{A} \mathbf{x}$  is called a quadratic form.  $\mathbf{x}^\mathsf{T} \mathbf{A} \mathbf{x} = \sum_i x_i (\mathbf{A} \mathbf{x})_i \\ = \sum_i x_i \left( \sum_j \mathbf{A}_{i,j} x_j \right) \\ = \sum_i \sum_j \mathbf{A}_{i,j} x_i \ x_j$  If  $\mathbf{A}$  is a diagonal matrix,  $\mathbf{x}^\mathsf{T} \mathbf{A} \mathbf{x} = \sum_i x_i (\mathbf{A} \mathbf{x})_i \\ = \sum_i x_i (\mathbf{A}_{i,i} \mathbf{x}_i) \\ = \sum_i x_i^2 \mathbf{A}_{i,i}$ 

Given a symmetric square

Also, recall from earlier:

- $\sum_{i} \mathbf{W}_{i,j} = \mathbf{D}_{i,i}$
- L = D W

### Laplacian Eigenmaps Beyond the Line

- How to find the embedding into m-dimensional space?
- The embedding is  $Y = [\mathbf{y}_1 \ \mathbf{y}_2 \ ... \ \mathbf{y}_m]$
- Minimize Objective function:

$$\sum_{ij} ||y^{(i)} - y^{(j)}||^2 W_{ij} = tr(Y^T L Y) \text{ i.e.}$$

$$\underset{\mathcal{V}}{\operatorname{argmin}} tr(Y^T L Y) \qquad \text{subject to} \quad Y^T L Y = I$$

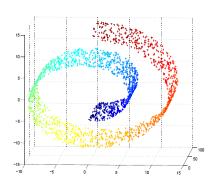
- Solution is provided by the matrix of eigenvectors corresponding to the lowest eigenvalues of the generalized eigenvalue problem Ly = λDy
- Ignore Zero Eigenvalue
  - In one-dimensional motivation, we imposed this as an additional constraint

### Laplacian Eigenmaps

- So each eigenvector is a function from nodes to ℝ in a way that "close by" points are assigned "close by" values.
- The eigenvalue of each eigenfunction gives a measure of how "close by" are the values of close by points
- By using the first m eigenfunctions for determining our m-dimensions we have our solution.

## Laplacian Eigenmap Example

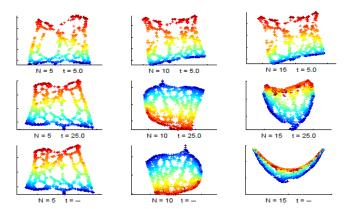
• Swiss roll



2000 random data points on the manifold

# Laplacian Eigenmap Example

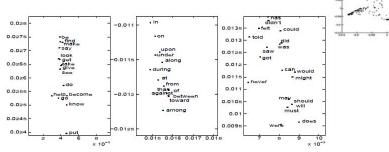
• 2D embedding of the swiss roll



Free parameters, N and t. N = Number of neighbors, t = Heat kernel parameter

### Laplacian Eigenmap Example

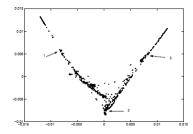
- 300 most frequent words from Brown corpus
- Each word is represented by a 600 dimensional vector
- Laplacian Eigenmap with N = 14, t = inf



Fragments labelled by arrows, from left to right. The first is exclusively infinites of verbs, the second contains prepositions and the third mostly modal and auxiliary verbs

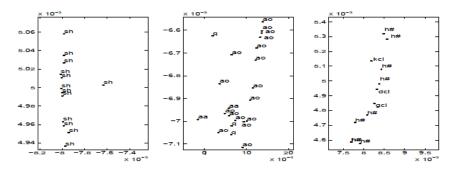
### Laplacian Eigenmap Example: Speech

- Speech signal is high dimensional but distinctive phonetic dimensions are few
- 30 ms window at 5 ms interval
- 256 Fourier coefficients for each 30 ms chunk
- 685 such vectors



685 speech data points plotted in the two dimensional Laplacian spectral representation

### Laplacian Eigenmap Example: Speech



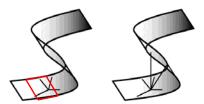
A blowup of the three selected regions. The data points corresponding to the same region have similar phonetic identity

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  - Laplacian Eigenmaps
  - Locally Linear Embedding
  - Isomap

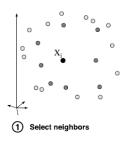
# Locally Linear Embedding (LLE) Sam T. Roweis, L. K. Saul 2000

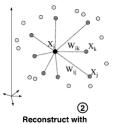
- Manifold Characteristics/Key Assumption
  - Provided there is sufficient data, we expect each data point and its neighbors to lie on or close to a locally linear patch



### **LLE Algorithm**

- Step 1:
  - Assign neighbors to each data point X<sub>i</sub>
- Step 2
  - Characterize the local geometry of linear patches by linear coefficients that reconstruct each point from its neighbors





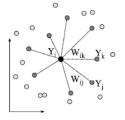
### **LLE Algorithm**

- Step 2: How to assign weights?
  - Minimize cost function measuring reconstruction error

- $\epsilon(W) = \sum_i |X_{i-} \sum_j W_{ij} X_j|^2$
- Weight W<sub>ij</sub> summarizes the contribution of the j<sup>th</sup> data point to the i<sup>th</sup> reconstruction
- Assign weights under two constraints
- $-W_{ij} = 0$  if  $X_i$  does not belong to set of neighbors of  $X_i$
- The rows of the weight matrix sum to one i.e.  $\Sigma_i W_{ii} = 1$
- Closed-form solution, Constrained Least Squares
   Problem (appendix A in paper)

### **LLE Algorithm**

- Step 3: Map to embedded coordinates
  - Each high-dimensional observation X<sub>i</sub> is mapped to a low-dimensional vector Y<sub>i</sub>
  - Choose Y<sub>i</sub> to minimize the embedding cost function



Map to embedded coordinates

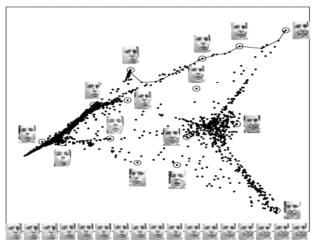
$$\Phi(Y) = \sum_{i} \left| \vec{Y}_{i} - \Sigma_{j} W_{ij} \vec{Y}_{j} \right|^{2}$$

- The cost function can be minimized (subject to constraints) by solving a sparse NxN eigenvalue problem (appendix B in paper).
  - •Bottom d non-zero eigenvectors

### **LLE Algorithm**

- The constrained weights obey an important symmetry
  - For a particular data point, the weights are invariant to rotation, rescaling and translation of the data point and its neighbors.
- The same weights that reconstruct the data points in D dimensions should reconstruct it in the manifold coordinate in d dimensions.
  - The weights characterize the intrinsic geometric properties of each neighborhood.

### LLE Example



Images of faces mapped into the embedding space described by the first two coordinates of LLE. Representative faces are shown next to circled points. The bottom images correspond to points along the top-right path (linked by solid line) illustrating one particular mode of variability in pose and expression.

### Effect of K

Require dense data points on the manifold for good estimation

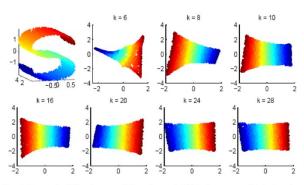


FIG. 5. S-curve (top left) and computed 2D coordinates by LLE with various neighborhood size k

### LLE and Laplacian Eigenmap

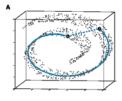
- LLE is connected with Laplacian Eigenmap
- LLE minimizes y<sup>T</sup>(I-W)<sup>T</sup>(I-W)y which reduces to finding eigenvectors of (I-W)<sup>T</sup>(I-W)
- They show that finding eigenvectors of (I-W)<sup>T</sup>(I-W) can be re-interpreted as finding eigenvectors of iterated Laplacian L<sup>2</sup>. Eigenvectors of L<sup>2</sup> coincide with those of L.

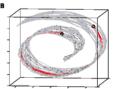
### Outline

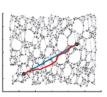
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### Isomap

Josh. Tenenbaum, Vin de Silva, John langford 2000

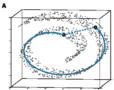


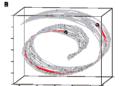


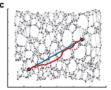


- Classical MDS uses Euclidean distance
- What we really want:
  - Distance measurements along manifold (geodesics)
  - Find low dimensional reconstruction which also has these geodesic distances
- Isomap: Classical MDS with geodesic distances.

# Isomap Algorithm Josh. Tenenbaum, Vin de Silva, John langford 2000



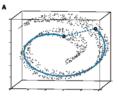


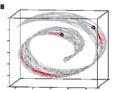


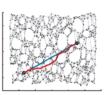
- Step 1: Construct Neighborhood graph (G)
  - Define the graph G over all data points by connecting points i and j if they are
    - Closer than  $\epsilon$  ( $\epsilon$ -Isomap)
    - If *i* is one of the k nearest neighbors of *j* (k-isomap)
  - Set edge lengths equal to  $d_x(i,j)$

### Isomap Algorithm

Josh. Tenenbaum, Vin de Silva, John langford 2000







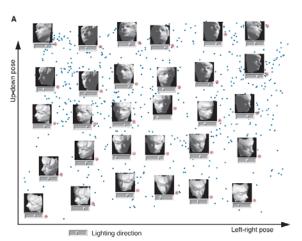
- Step 2: Compute Shortest Paths in G
  - Floyd's algorithm (O(n³)) or Dijkstra's algorithm to find D<sub>G</sub>
- Step 3: Construct d-dimensional embedding
  - Apply classical MDS on D<sub>G</sub> to find d-dimensional embedding

### Isomap

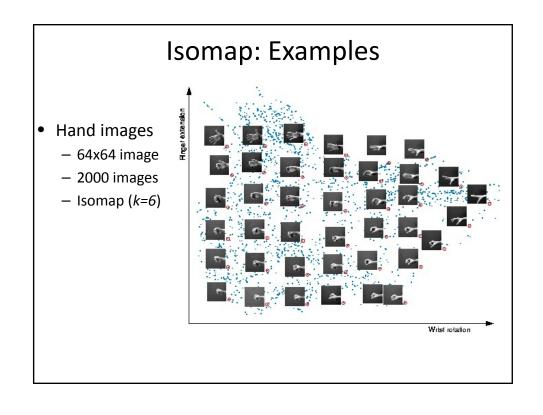
- Advantages
  - Non-linear. Preserves intrinsic geometry of the data.
  - Non-iterative polynomial time algorithm
  - Guarantee of global optimality
    - For intrinsically Euclidean manifolds, a guarantee of asymptotic convergence to the true structure
    - · the ability to discover manifolds of arbitrary dimensionality
- Disadvantages
  - From Wikipedia
    - "short-circuit errors" from noise or if k is too large.
    - "Even a single short-circuit error can alter many entries in the geodesic distance matrix, which in turn can lead to a drastically different (and incorrect) low-dimensional embedding"

### Isomap: Examples

- Dimensionality reduction for visual perception
  - 64x64 image
  - 698 raw images
  - Isomap (k=6)



# Isomap: Examples • Handwritten '2' -1000 handwritten 2s $-1 \text{ Isomap } (\epsilon=4.2)$



### **Residual Variance** Residual Variance 0.6 $= 1 - \rho(D_m, D_v)^2$ 0.5 • where $\rho$ is the correlation 0.15 Face Images SwisRoll coefficient operator 0.3 0.1 D<sub>m</sub> contains **estimated** 0.2 0.05 distances between data in the original space and D<sub>v</sub> contains distances between data points in 0.5 C D projected space 0.4 Residual Variance is zero if 0.6 Hand Images 0.3 estimated distances between 0.4 points in high dimensional 0.2 space is perfectly correlated with distances between corresponding points in Dimension projected space.

### Isomap Vs LLE

- Isomap
  - 1. MDS on the geodesic distance matrix
  - 2. Global approach
- LLE
  - 1. Model local neighborhoods as linear patches and then embed in a lower dimensional manifold.
  - 2. Local approach
  - 3. Computationally efficient. Eigenvectors from sparse matrices

### **Graph Kernels**

- •We Considered Two Variations for Weighting Edges for the Laplacian Eigenmap Algorithm
  - Heat Kernel

$$\mathbf{W}_{ij} = e^{\frac{-\left\|x_i - x_j\right\|^2}{t}}$$
 if i and j connected, 0 otherwise

– Simple-Minded

 $\mathbf{W}_{ij} = 1$  if i and j connected, 0 otherwise

- Overview of Additional Graph Kernels
  - Diffusion Kernel

$$\mathbf{K}_{ij} = \left[\sum_k rac{\lambda^k}{k!} \mathbf{A}^k\right]_{ij} = \left[\min(\lambda \mathbf{A})\right]_{ij}$$
 if i and j connected, 0 otherwise

**A** is the adjacency matrix. Discounts a k-length walk by  $\frac{\lambda^k}{k!}$  for  $0 \leq \lambda \leq 1$ 

- Resistance Kernel

(also called the commute-time kernel)

$$K = (D - A)^+$$

A is the adjacency matrix, and D is the degree matrix,

and + is the Moore-Penrose pseudoinverse operator.

Interprets a graph as a network of resistance, where edge weights are interpreted relative to resistance values in an electrical network.

### **Summary**

- Isomap, LLE and Laplacian Eigenmap: Non-linear dimensionality reduction technique
- Useful for learning manifolds, understanding low dimensional data embedded in high dimensional space.
- PCA and MDS fails for this type of data.
- All three use some technique to preserve local geometry i.e. inter-point relationships

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### Additional Laplacian Eigenmaps Details

### Continuous Manifold

- Laplacian of a graph is analogous to the Laplace Beltrami operator on manifolds.
- Mapping to 1-D. Find a map f such that points close together on the manifold get mapped close together on the line.
- Two points z and x mapped to f(z) and f(x). It is shown that

$$|f(\mathbf{z}) - f(\mathbf{x})| \le \|\nabla f(\mathbf{x})\| \ \|\mathbf{z} - \mathbf{x}\| + o\left(\|\mathbf{z} - \mathbf{x}\|\right)$$

# Additional Laplacian Eigenmaps Details Continuous Manifold

- Gradient of f provides us with an estimate of how far apart f maps nearby points.
- Minimizing the gradient minimizes the values assigned to close by points.

$$\underset{\|f\|_{L^2(\mathcal{M})}=1}{\operatorname{argmin}} \int_{\mathcal{M}} \|\nabla f(x)\|^2$$

• Minimizing the objective function reduces to finding eigenfunctions of the Laplace Beltrami Operator