Dimension Reduction

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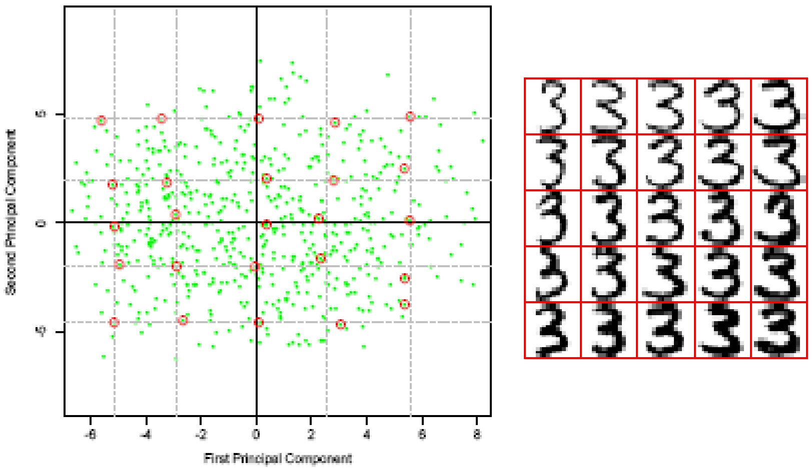
Introduction

- Goal: choosing suitable transforms, so as to obtain high "information packing".
  - Raw data -> Meaningful features.
  - Unsupervised/Automatic methods.

- To exploit and remove information redundancies via transform.

Feature extraction

- Data independent
  - DFT, DWT, DCT
    - A single piece of signal



- Data dependent
  - PCA, K-PCA, ICA, ISO-MAP, LLE …
    - A set of signals (images, motion data, shapes,…)

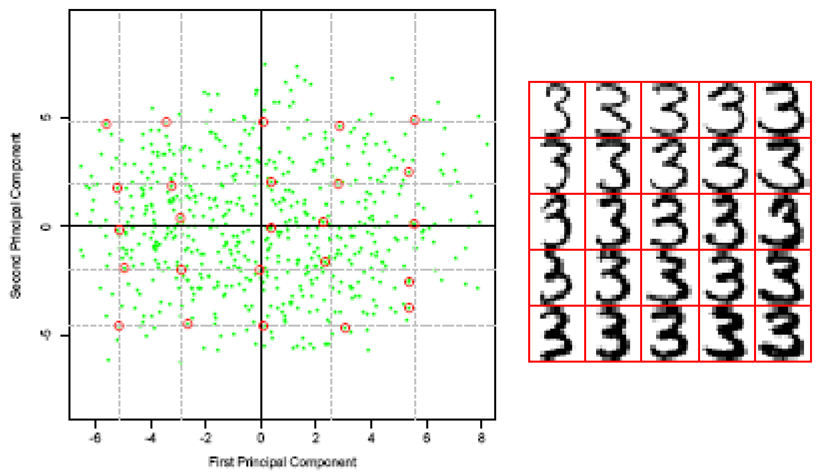
- Key: define desirable transforms
  - Raw data -> Feature space

PCA: example
Digit data

$$X = \begin{pmatrix} x_{0,0} & x_{1,0} & x_{2,0} & \cdots & x_{N-1,0} \\ x_{0,1} & x_{1,1} & x_{2,1} & \cdots & x_{N-1,1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{0,p-1} & x_{1,p-1} & x_{2,p-1} & \cdots & x_{N-1,p-1} \end{pmatrix}_{N \times p}$$

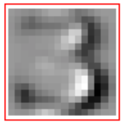
130 threes, a subset of 638 such threes and part of the handwritten digit dataset. Each three is a 16 $\times$ 16 greyscale image, and the variables Xj, j = 1, . . . , 256 are the greyscale values for each pixel.

Digit:
rank-2 model for threes



Two-component model has the form

$$\hat{f}(\lambda) = \bar{x} + \lambda_1 v_1 + \lambda_2 v_2$$

$=$  $+ \lambda_1 \cdot$  $+ \lambda_2 \cdot$ .

Here we have displayed the first two principal component directions, v_1 and v_2, as images.

Principal Components

- Suppose we have N measurements on each of p variables X_j, $j=1,2,\ldots,p$. There are several equivalent approaches to principal components:
  - Produce a derived (and small) set of uncorrelated variables $Z_k = a_k^T X, k = 1,\ldots,q < p$ that are linear combinations of the original variables, and that explain most of the variation in the original set.
  - Approximate the original set of *N* points in $\Re^p$ by a least-squares optimal linear manifold of co-dimension $q < p$.
  - Approximate the $q < p$ data matrix $\boldsymbol{X}$ by the best rank-q matrix $\hat{\boldsymbol{X}}(p)$. This is the usual motivation for the SVD.

数据的简化线性表示

数据的低维线性流形近似

矩阵逼近

Basis Vectors and Images

- Input samples

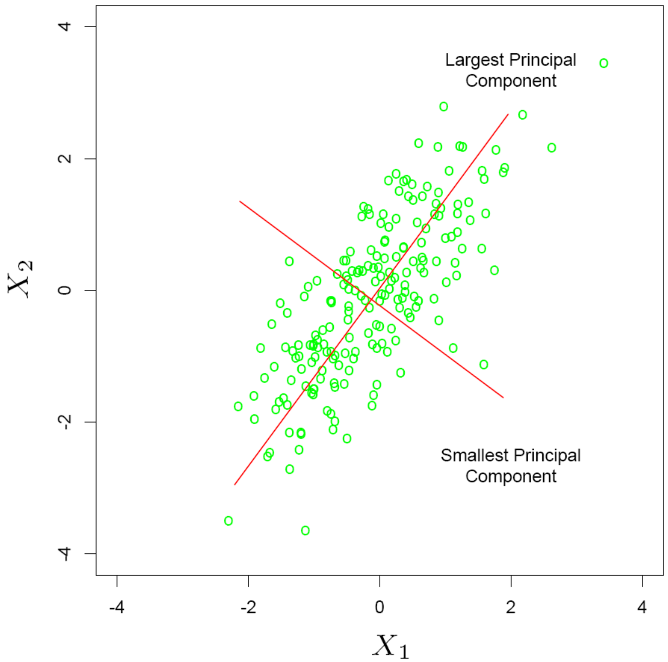
$$\mathbf{X}^T = [X(1), X(2), \ldots, X(p)]$$

- Unitary $p \times p$ matrix A and transformed Vector $\mathbf{Z} = \mathbf{AX}$
- Basis vector representation

$$\mathbf{x} = \mathbf{Az} = \sum_{i=0}^{N-1} z(i)\mathbf{a}_i$$

$$< \mathbf{a}_j, \mathbf{x} > = \mathbf{a}_j^T \mathbf{x} = \sum_{i=1}^{p} z(i) < \mathbf{a}_j, \mathbf{a}_i > = z(j)$$

PCA: Derived Variables



$$\Sigma = X^T X$$

- $Z_1 = a_1 X$ is the projection of the data onto the longest direction, and has the largest variance amongst all such normalized projections.
- α_1 is the largest eigenvalue of Σ, the sample covariance matrix of X. Z_2 and α_2 correspond to the second-largest eigenvector.

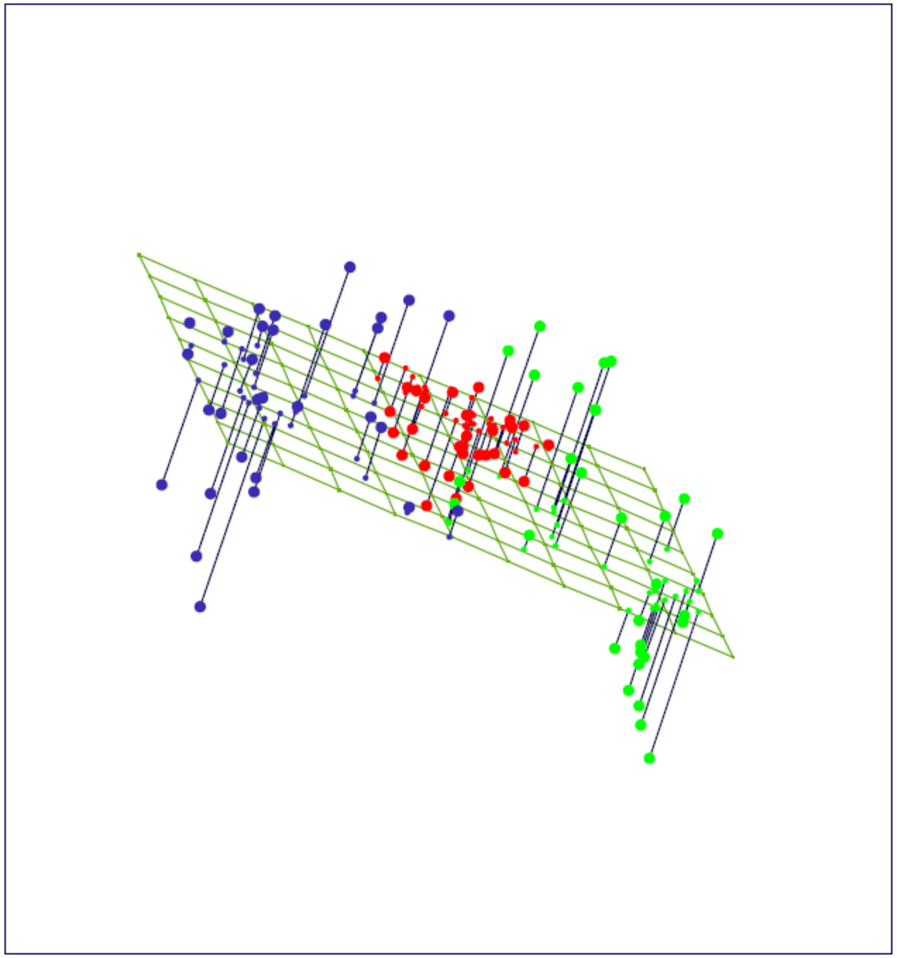
PCA: Least Squares Approximation

Find the linear manifold

$$f(\lambda) = \mu + \mathbf{V}_q \lambda$$

that best approximates the data in a least-squares sense:

$$\min_{\mu,\{\lambda_i\},\mathbf{V}_q} \sum_{i=1}^{N} \left\| \boldsymbol{x}_i - \mu - \mathbf{V}_q \lambda_i \right\|^2$$



Solution:

$$\mu = \bar{x}, v_k = a_k, \lambda_k = Z_k$$

PCA:
Singular Value Decomposition

Let $\hat{X}$ be the centered $N \times p$ data matrix (assume $N > p$).

Singular values

$$\boldsymbol{X} = \begin{pmatrix} x_{0,0} & x_{1,0} & x_{2,0} & \cdots & x_{N-1,0} \\ x_{0,1} & x_{1,1} & x_{2,1} & \cdots & x_{N-1,1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{0,p-1} & x_{1,p-1} & x_{2,p-1} & \cdots & x_{N-1,p-1} \end{pmatrix}_{N \times p} = \boldsymbol{USV}$$

x_1

Unitary Matrices

is the SVD of $\hat{X}$, where

- ***U*** **is *N*×*p* orthogonal, the left singular vectors.**
- ***V*** **is *p*×*p* orthogonal, the right singular vectors.**
- ***S*** **is diagonal, with $d_1 \geq d_2 \geq \ldots \geq d_p \geq 0$, the singular values.**

✓ **The SVD always exists, and is unique up to signs. The columns of V are the principal components, and $Z_j = U_j d_j$.**

PCA: Singular Value Decomposition

Singular values

$$\boldsymbol{X} = \begin{pmatrix} x_{0,0} & \boxed{x_{1,0}} & x_{2,0} & \cdots & x_{N-1,0} \\ x_{0,1} & x_{1,1} & x_{2,1} & \cdots & x_{N-1,1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{0,p-1} & x_{1,p-1} & x_{2,p-1} & \cdots & x_{N-1,p-1} \end{pmatrix}_{N\times p} = \boldsymbol{USV}$$

x_1

Unitary Matrices

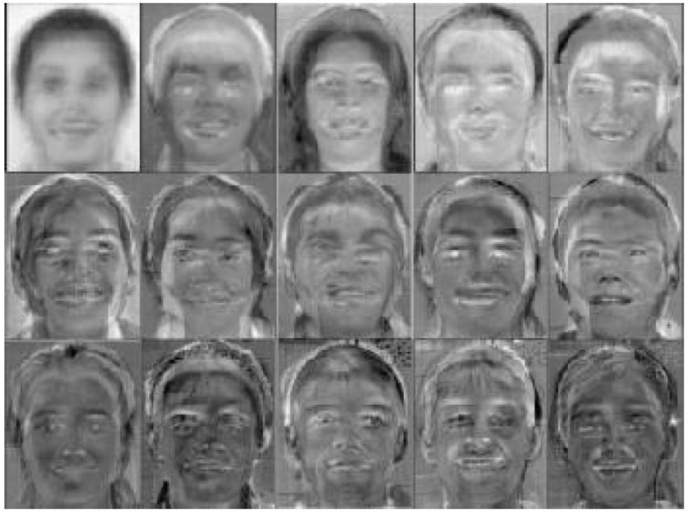
Eckart–Young theorem

Let s_q be s with all but the first q diagonal elements set to zero. Then $\hat{x}_q = \boldsymbol{U}s_q\boldsymbol{V}^T$ solves

$$\min_{rank(\hat{\boldsymbol{X}}_q)=q} \left\| \hat{\boldsymbol{X}} - \hat{\boldsymbol{X}}_q \right\|$$

PCA: example Eigenfaces

- G. D. Finlayson, B. Schiele & J. Crowley. Comprehensive colour image normalization. ECCV 98 pp. 475~490.

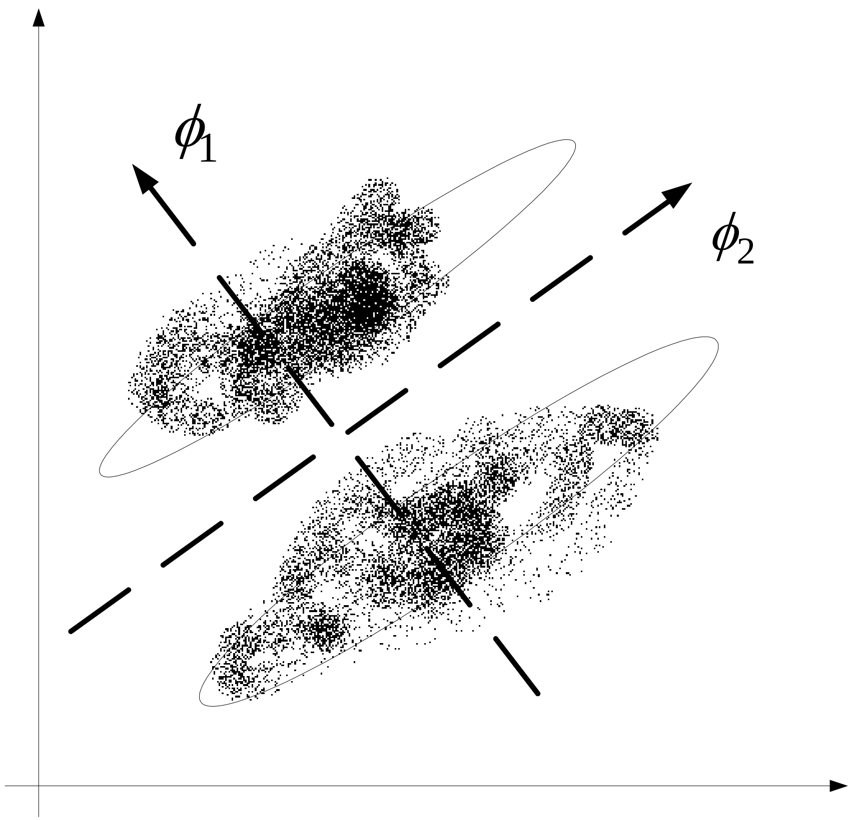


- Eigen-X, ☺

PCA and dimensional reduction

- Space transform via SVD
  - $X \rightarrow Y$
- Dimension:
  - $p >> q$
- Representation
- Errors …

Problems of PCA



- Only suitable for normal distributed data
- More consideration
  - ICA: Independent components.
  - K-PCA: Nonlinear
  - …

Nonlinear dimension reduction algorithms:

- Locally Linear Embedding (LLE), *Science*

  Sam T. Roweis and Lawrence K. Saul

- A Global Geometric Framework for Nonlinear Dimensionality Reduction (Isomap), *Science*

  Joshua B. Tenenbaum, Vin de Silva, John C. Langford

- BoostMap: A Method for Efficient Approximate Similarity Rankings, *CVPR 2004*

  Vassilis Athitsos, Jonathan Alon, Stan Sclaroff, and George Kollios

Locally Linear Embedding (LLE)

- Recovers global nonlinear structure from locally linear fits.
- Each data point and it's neighbors is expected to lie on or close to a locally linear patch.
- Each data point is constructed by it's neighbors:

$$\vec{\hat{X}}_i = \sum_j W_{ij} \vec{X}_j$$

$$W_{ij} = 0 \text{ if } \vec{X}_j \text{ is not a neighbor of } \vec{X}_i$$

LLE: Getting the Reconstruction Weights

- We want to minimize the error function:

$$\varepsilon(W) = \sum_i \left| \vec{X}_i - \sum_j W_{ij} \vec{X}_j \right|^2$$

- With the constrains:

$$W_{ij} = 0 \quad \text{if } \vec{X}_j \text{ is not a neighbor of } \vec{X}_i$$

$$\sum_j W_{ij} = 1$$

- Solution (using Lagrange multipliers):

$$W_j = \sum_k C_{jk}^{-1} (\vec{X}\vec{\eta}_k + \lambda)$$

$$\lambda = 1 - \sum_{jk} C_{jk}^{-1} (\vec{X}\vec{\eta}_k) \Big/ \sum_{jk} C_{jk}^{-1}$$

LLE: Find Embedded Coordinates

- Choose d-dimensional coordinates, Y, to minimize: $\phi(Y) = \sum_i \left| \vec{Y}_i - \sum_j W_{ij} \vec{Y}_j \right|^2$

  Under: $\sum_i \vec{Y}_i = \vec{0}, \quad \frac{1}{N} \sum_i \vec{Y}\vec{Y}^T = I$

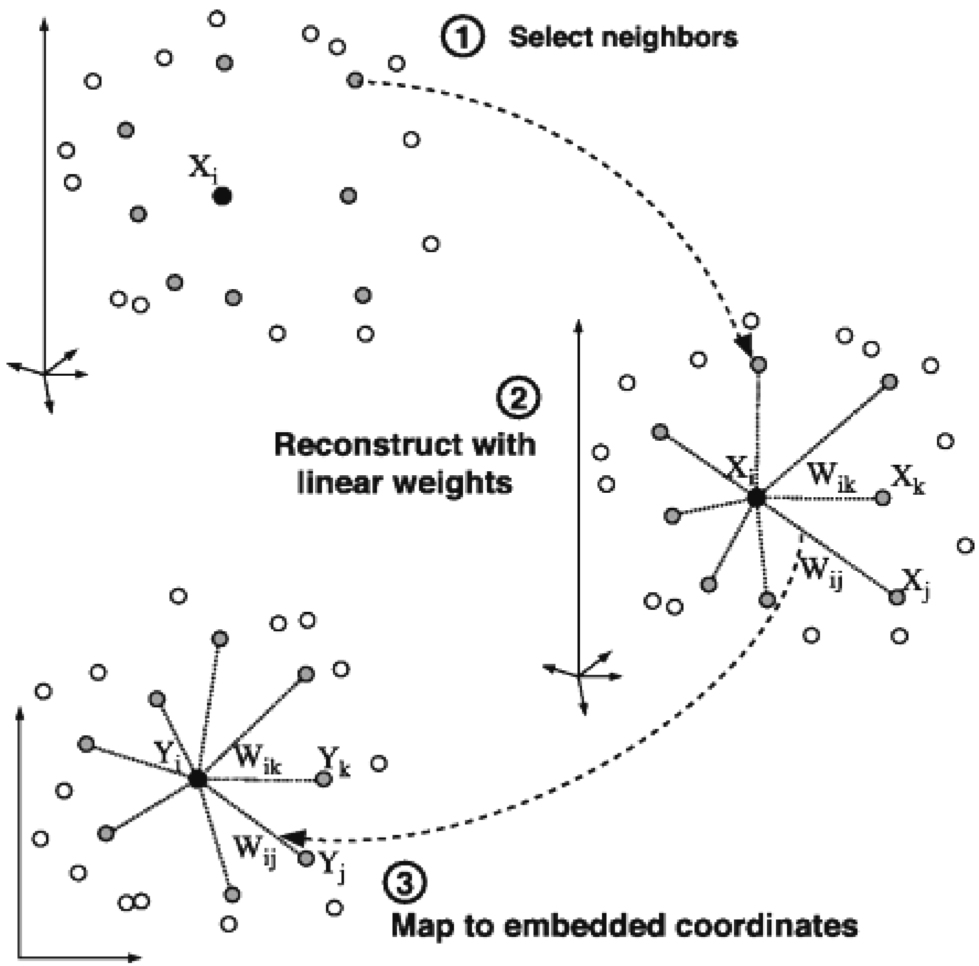
Quadratic form: $\phi(Y) = \sum_{ij} M_{ij} (\vec{Y}_i \vec{Y}_j)$

where: $M = (I - W)^T (I - W)$

- Solution: compute bottom d+1 eigenvectors of M. (discard the last one)

LLE: Summary

- Input: N data items in D dimension (X).
- Output: d < D dimensional embedding coordinates (Y) for the input points.



LLE:
Algorithm Pseudocode (I)

```
Find neighbors in X space
For i=1:N
    compute the distance from Xi to every other point Xj
    find the K smallest distances
    assign the corresponding points to be neighbors of Xi
end
```

http://www.cs.toronto.edu/~roweis/lle/algorithm.html

LLE: Algorithm Pseudocode (II)

Solve for reconstruction weights W.

for i=1:N

    create matrix Z consisting of all neighbors of Xi
    subtract Xi from every column of Z

    compute the local covariance C=Z'*Z

    solve linear system C*w = 1 for w

    set Wij=0 if j is not a neighbor of I

    set the remaining elements in the ith row of W equal to w/sum(w);

end

LLE: Algorithm Pseudocode (III)

Compute embedding coordinates Y using weights W.

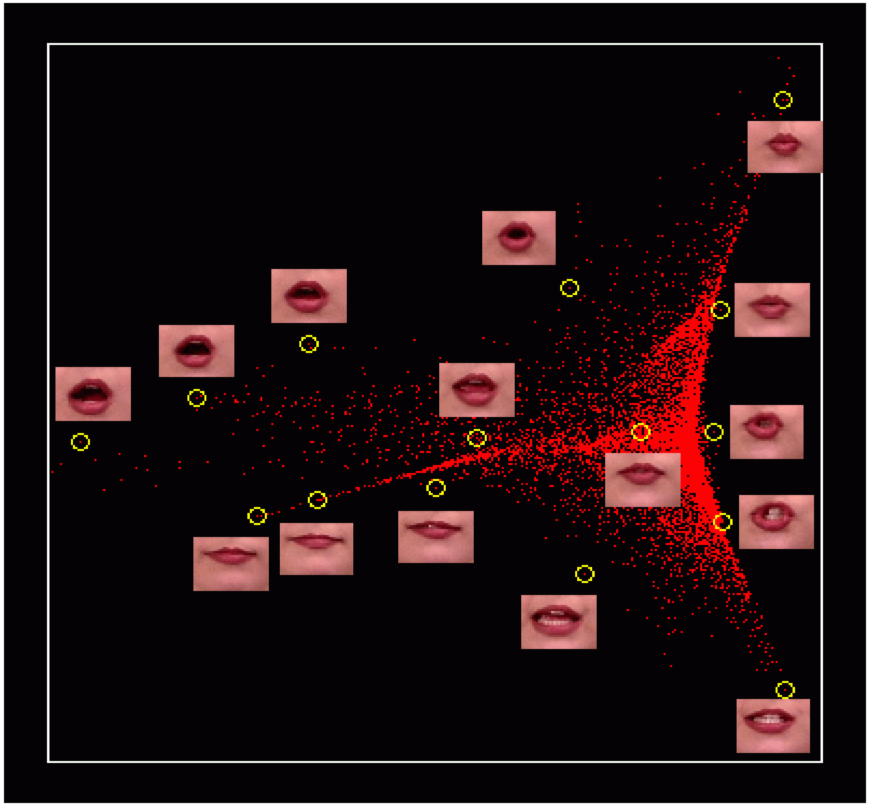
create sparse matrix M = (I-W)'*(I-W)

find bottom d+1 eigenvectors of M (corresponding to the d+1 smallest eigenvalues)

set the *q*-th ROW of Y to be the *q*+1 smallest eigenvector (discard the bottom eigenvector [1,1,1,1...] with eigenvalue zero)

LLE: Example

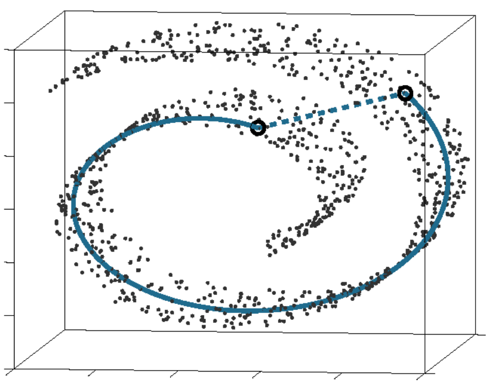
- N=8588 (RGB) images of lips of size 108x84. D=27216
- Num of neighbors K=16

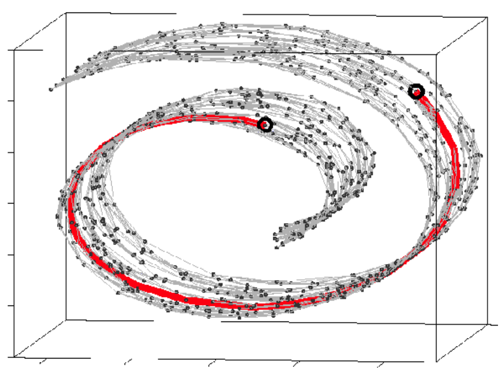


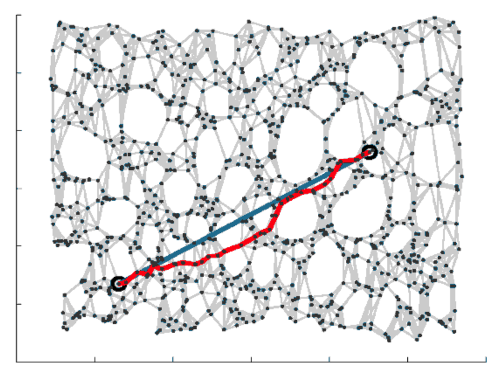
Isomap: (Science 2001) Isometric feature mapping

- Preserve the intrinsic geometry of the data.
- Use the geodesic manifold distances between all pairs.

Three steps algorithm

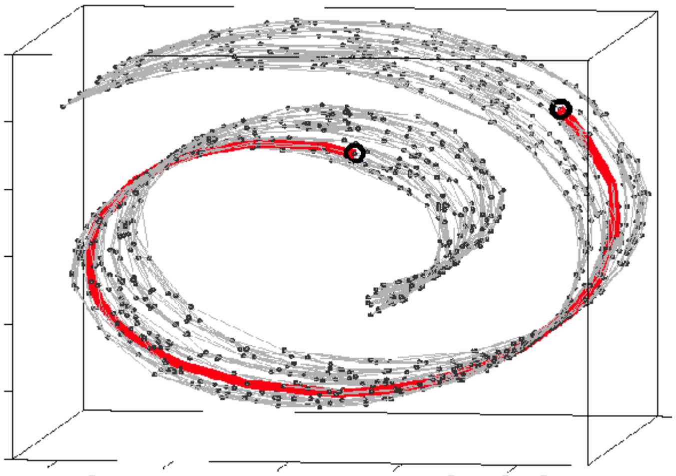






Isomap: Construct Neighborhood Graph

- Determine which points are neighbors, based on the distances d(i,j) .
  - K nearest neighbors
  - ε-radius

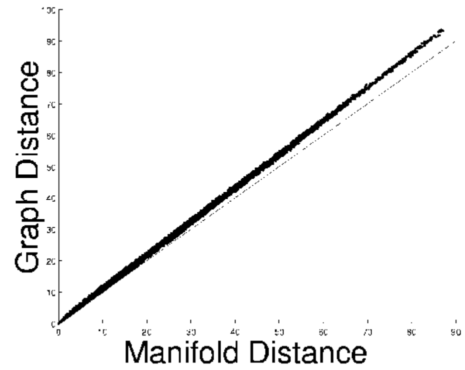


- Create a graph G, with edges between neighbors and distance weights.

Isomap: Compute Shortest Paths

- Estimate the geodesic distances.
- Compute all-pairs shortest paths in G.
- Can be done using Floyd's algorithm, $O(N^2 \ln N)$.

$$d_G(i,j) = d(i,j) \quad \text{neighboring } i, j$$
$$d_G(i,j) = \infty \qquad \text{othewise}$$



$$\textit{for } \mathrm{k} = 1,2,\ldots,\mathrm{N}$$
$$d_G(i,j) = \min\{\, d_G(i,j),\ d_G(i,k) + d_G(k,j)\}$$

Isomap:
Construct d-dimensional Embedding

Classical MDS with $d_G(i,j)$,
minimize the cost function:

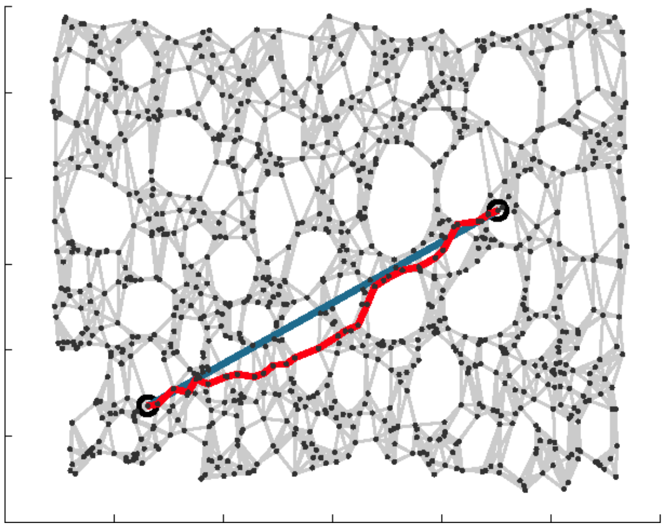
$$E = \left\| \tau(D_G) - \tau(D_Y) \right\|_{L^2}$$

$$\textit{where } D_Y(i,j) = \left\| y_i - y_j \right\|$$

$$D_G(i,j) = d_G(i,j)$$

and

$$\tau(D) = \tfrac{-1}{2}(I - \tfrac{1}{N}) D^{\cdot 2} (I - \tfrac{1}{N})$$



Solution: take top d eigenvectors of the matrix $\tau(D_G)$

Isomap:
Classical Multi-dimensional Scaling

$$\mathbf{X'X} = -\frac{1}{2}\mathbf{JEJ}$$

E: Euclidian distance matrix

$$\mathbf{B} = -\frac{1}{2}\mathbf{JMJ}$$

M: Manifold distance matrix

$$L(\hat{\mathbf{X}}) = \left\| -\frac{1}{2}\mathbf{J}\left(\mathbf{E}-\mathbf{M}\right)\mathbf{J} \right\| = \left\| \hat{\mathbf{X}}\hat{\mathbf{X}}' - \mathbf{B} \right\|.$$

$$\mathbf{B} = \mathbf{Q}\Lambda\mathbf{Q}' \qquad \hat{\mathbf{X}} = \mathbf{Q}_+\Lambda_+^{\frac{1}{2}}$$

$$c_i = \sum_{a=1}^{m} x_{ia}^2$$

$$d_{ij}^2 = \sum_{a=1}^{m} (x_{ia} - x_{ja})^2$$

$$\mathbf{E} = \mathbf{c}\mathbf{1}' + \mathbf{1}\mathbf{c}' - 2\mathbf{XX}'$$

$$\mathbf{J} = \mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}'$$

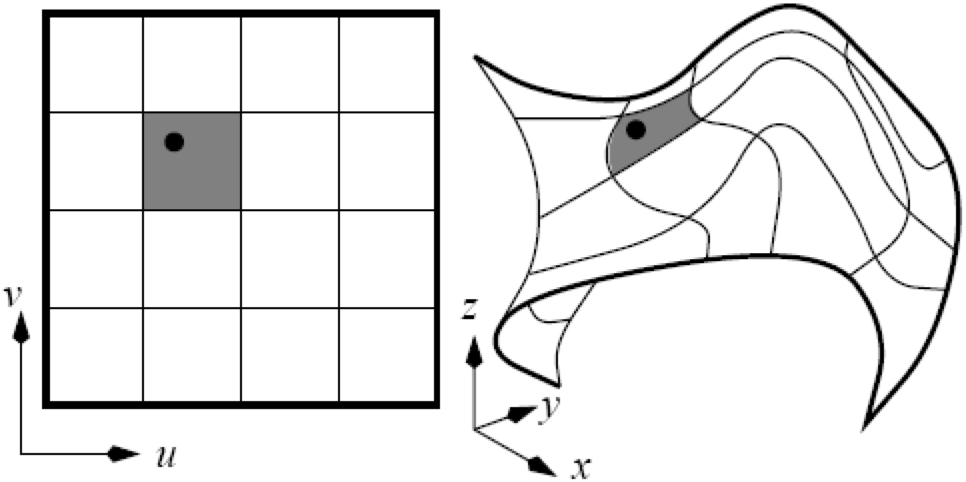
$$\begin{aligned} \mathbf{B} &= -\frac{1}{2}\mathbf{J}(\mathbf{c}\mathbf{1}' + \mathbf{1}\mathbf{c}' - 2\mathbf{XX}')\mathbf{J} \\ &= -\frac{1}{2}\mathbf{J}\mathbf{c}\mathbf{0}' - \frac{1}{2}\mathbf{0}\mathbf{c}'\mathbf{J} + \mathbf{JXX}'\mathbf{J} \\ &= \mathbf{XX}'. \end{aligned}$$

Eigen-structure analysis, SVD again

Isomap:
Classical Multi-dimensional Scaling (2D)

$$
\begin{aligned}
\mathbf{J} &= \mathrm{eye}(n) - \mathrm{ones}(n)./n; \\
\mathbf{B} &= -0.5 * \mathbf{J} * \mathbf{M} * \mathbf{J}; \\
& \quad \text{\% Find largest eigenvalues+their eigenvectors:} \\
[\mathbf{Q}, \mathbf{L}] &= \mathrm{eigs}(\mathbf{B}, 2, \text{'LM'}); \\
& \quad \text{\% Extract the coordinates:} \\
\mathrm{newy} &= \mathrm{sqrt}(\mathbf{L}(1,1)). * \mathbf{Q}(:,1); \\
\mathrm{newx} &= \mathrm{sqrt}(\mathbf{L}(2,2)). * \mathbf{Q}(:,2);
\end{aligned}
$$

Isomap: application texture mapping



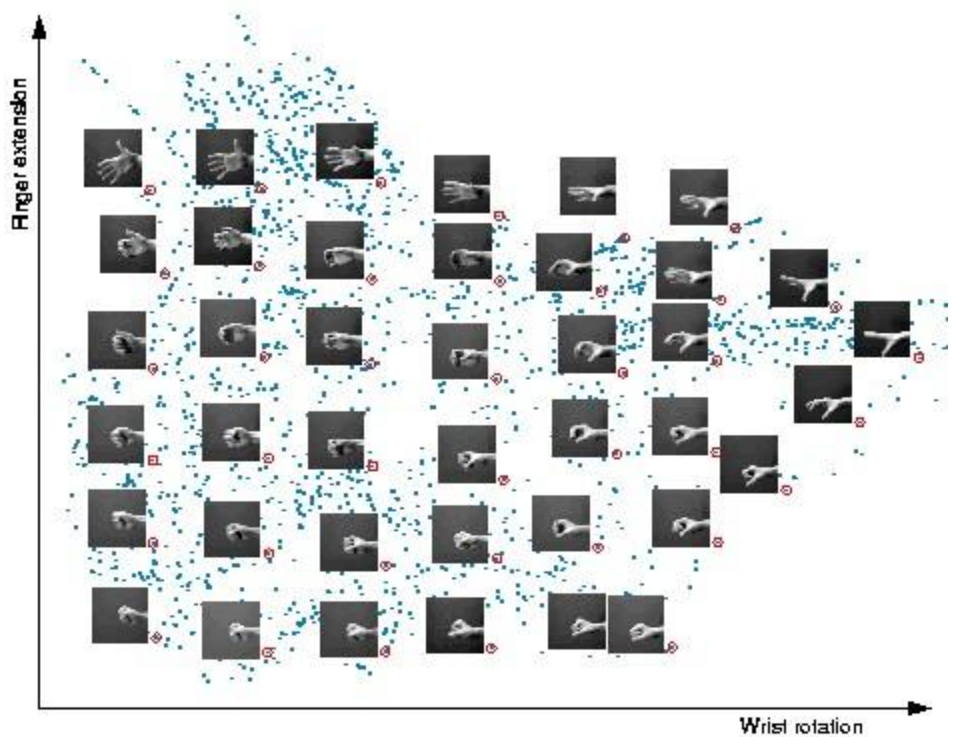
(a) (b)

Fig. 3. An example of a face flattening. (a) A 3D reconstruction of a face. (b) The flattened texture image of the face.

(a) (b)

Isomap: Examples

- *N*=2000 images
  64x64 pixels K=6

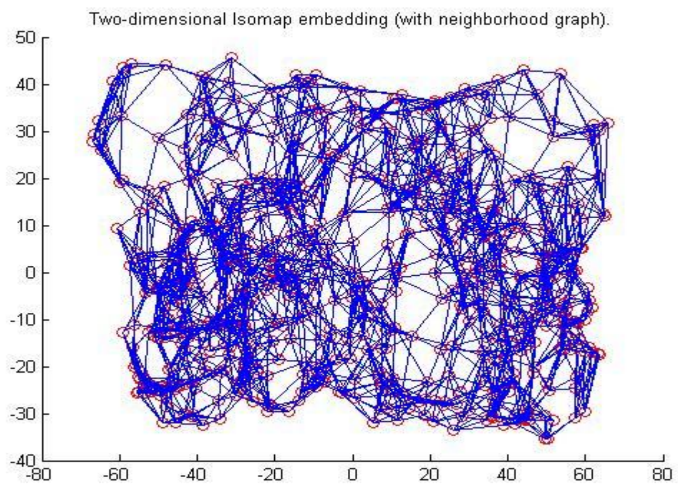


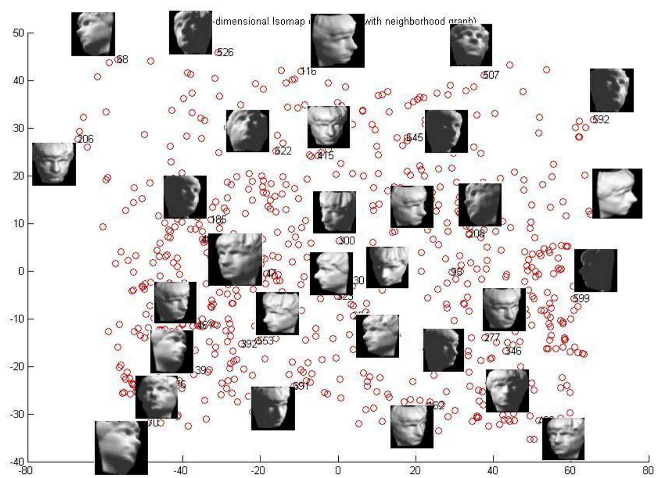
Isomap: More Results

Input: 698
images of 64x64

K=7, d=2

Outputs:

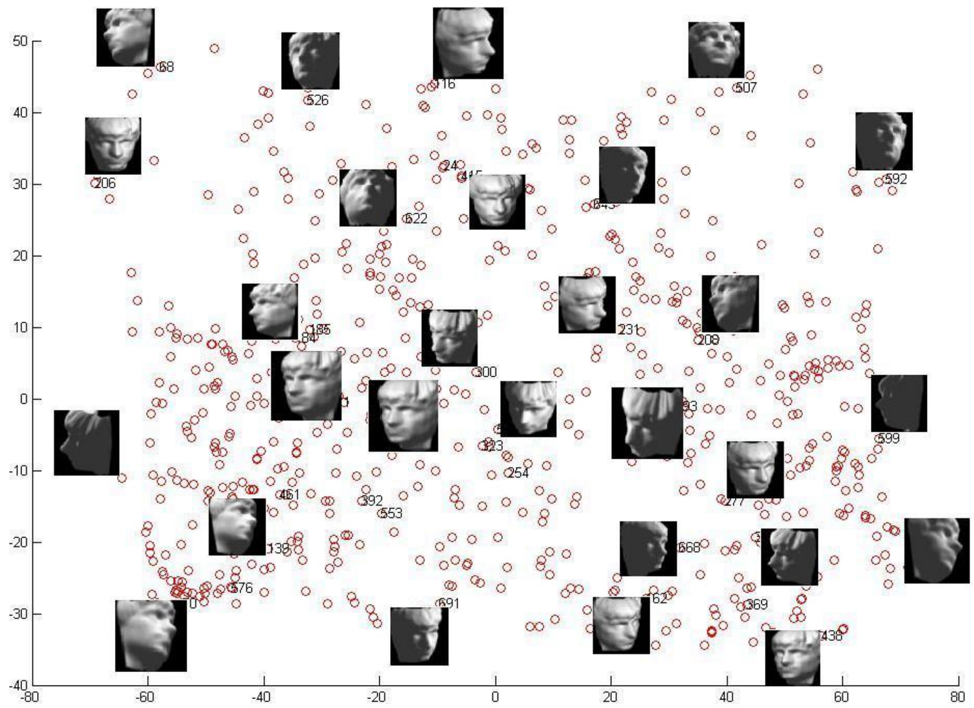




Isomap:
More Results

- Same inputs, but this time with d=3

698 images of 64x64 K=7



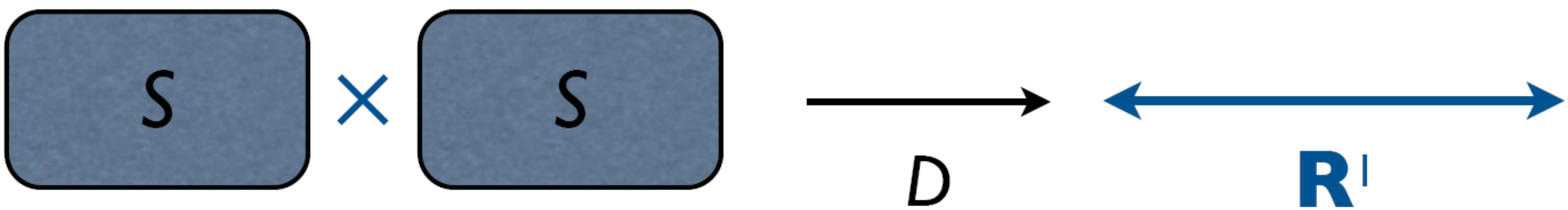
BoostMap:
A different perspective of embedding

- Goal – Significantly reduce retrieval time in image database systems.

- Embedding is formulated as a machine learning task.
- AdaBoost is used to combine many simple 1D embeddings into a d-dimensional embedding.
- Obtain ranking of all DB objects in order of similarity to a query object.

BoostMap: main idea

Data Set S, Distance function $D: S \times S \rightarrow \mathbf{R}^1$



Main Points:

- D may be expensive to compute.
- D may not satisfy triangle inequality.

BoostMap: Problem Definition

- Embeddings are seen as classifiers.
- Estimate for *a, b, c* if *a* is closer to *b* or *c*.
- X – set of objects
- D_X – distance measure.

$$P_X(q, x_1, x_2) = \begin{cases} 1 \text{ if } \mathrm{D_X}(q, x_1) < \mathrm{D_X}(q, x_2) \\ 0 \text{ if } \mathrm{D_X}(q, x_1) = \mathrm{D_X}(q, x_2) \\ -1 \text{ if } \mathrm{D_X}(q, x_1) > \mathrm{D_X}(q, x_2) \end{cases}$$

- Find an Embedding F: X → R^d and a measure D_{R^d} that is used for evaluating any triplet.

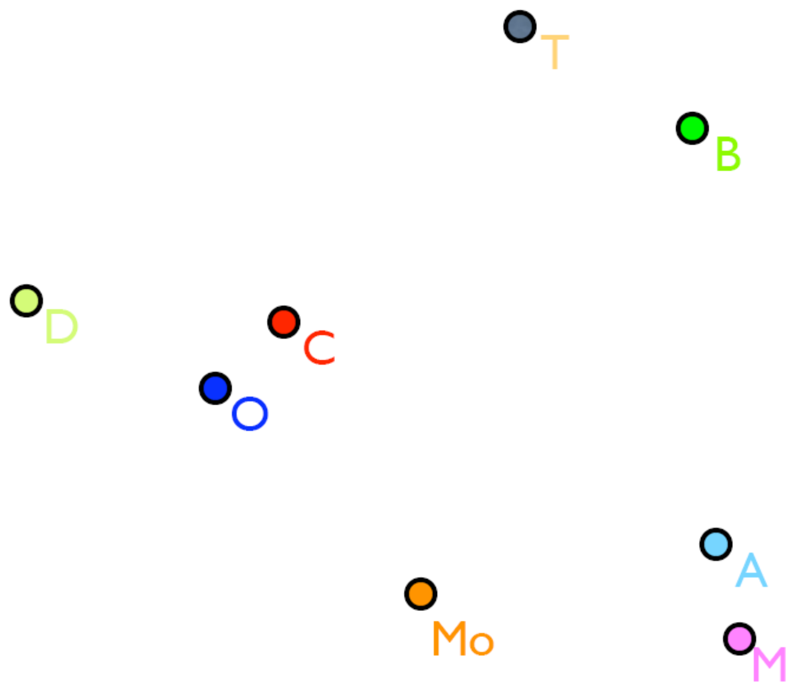
$$\widetilde{F}(q, x_1, x_2) = D_{R^d}(F(q), F(x_2)) - D_{R^d}(F(q), F(x_1))$$

- Data Set S, Distance function $D : S \times S \rightarrow \mathbf{R}^l$
- Proximity function $P(r; x,y) = \mathrm{sgn}(\ D(y,r) - D(x,r)\ )$

Example.

Some proximity function values for "Cities of North America"

Cities of North America



BoostMap - Outputs

- The output is a classifier: $H = \sum_{j=1}^{d} \alpha_j \widetilde{F}_j$

- The final output is an embedding F : X → R^d

  And a distance measure D : R^d xR^d → R^d

$$F(x) = \left(F_1(x), \ldots, F_d(x)\right)$$

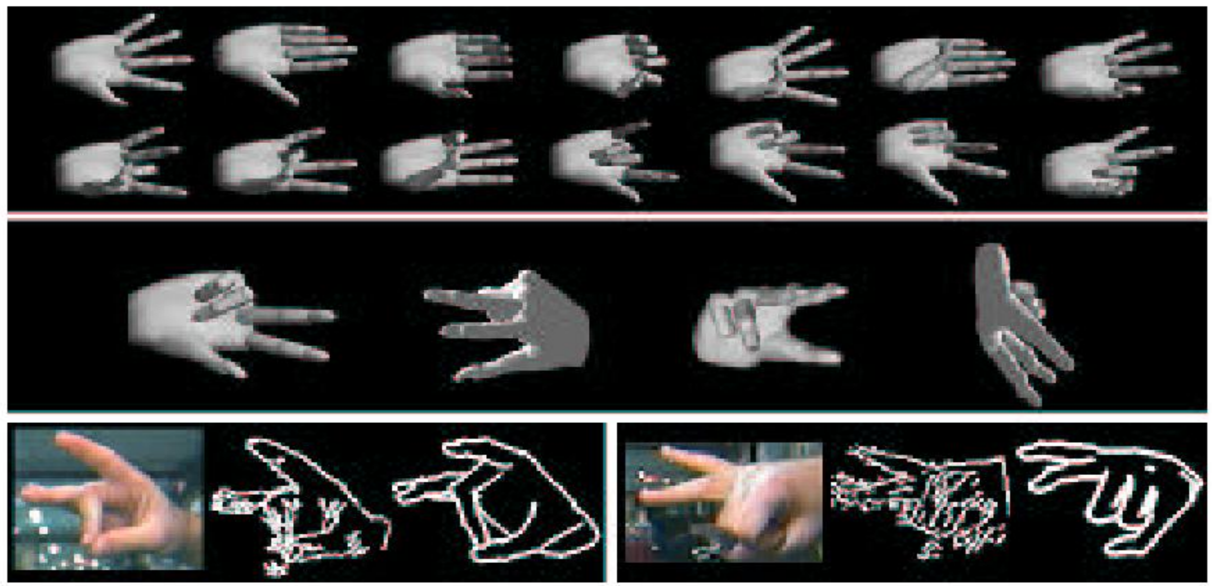
$$D_{R^d}\left((u_1, \ldots, u_d), (v_1, \ldots, v_d)\right) = \sum_{j=1}^{d} \left(\alpha_j \left| u_j - v_j \right|\right)$$

BoostMap - Results

Hand shapes used in the training set

Orientations used in the training set

Retrieval results



original

The query

Correct match

Summary:
Nonlinear Dimensionality Reduction

- **Isomap - Use the geodesic manifold distances between all pairs.**
  - **sees more than just the Euclidean structure.**
  - **polynomial time procedure.**

- **LLE - Recovers global nonlinear structure from locally linear fits.**
  - **no need no estimate pair-wise distances.**
  - **optimization do not involve local minima.**

- **BoostMap - looks at embeddings as classifiers, uses AdaBoost.**
  - **main usage: similarity retrieval from database.**
  - **main advantage: trained offline, applicable online.**
- Manifold learning …

流形学习法

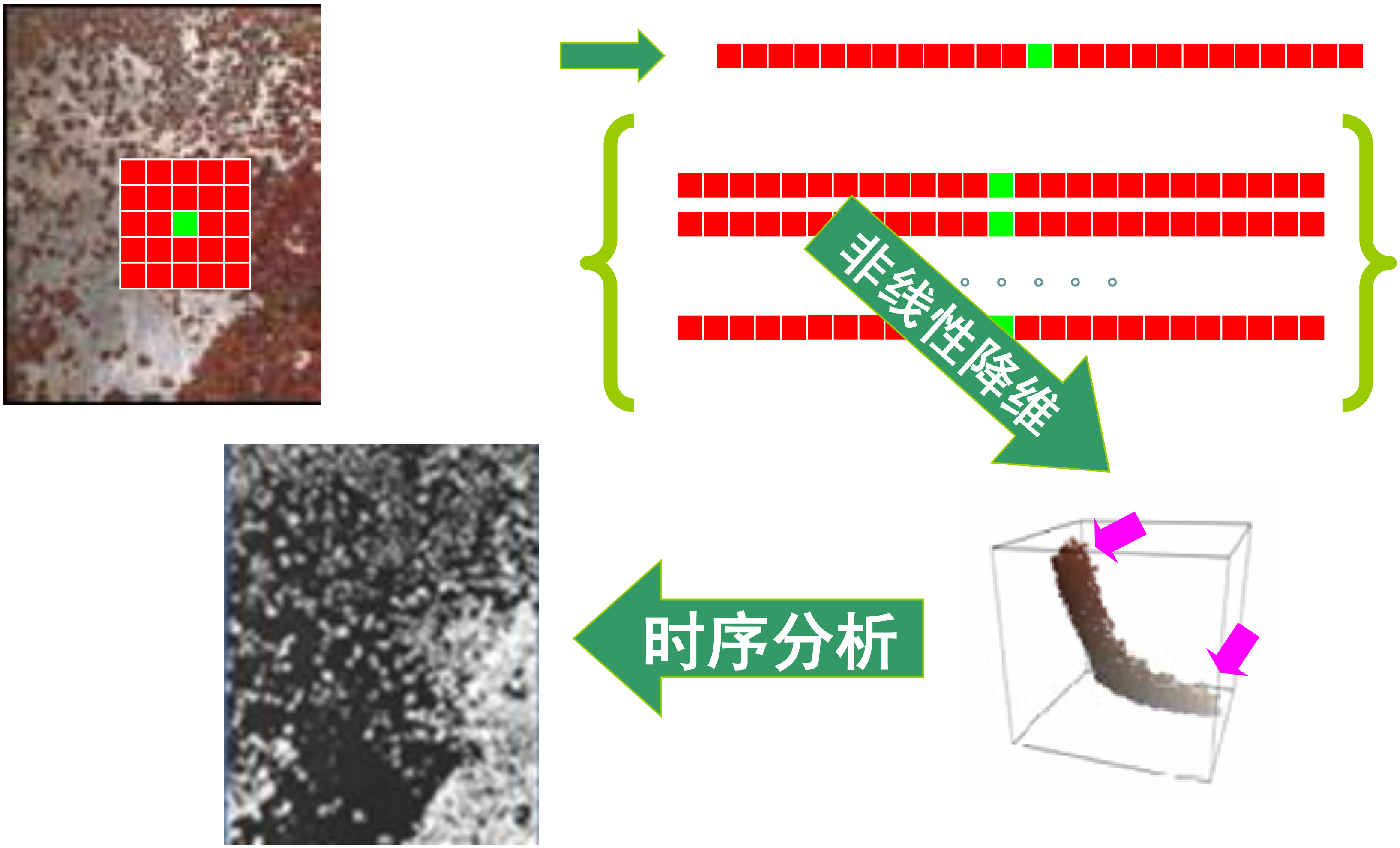
- 关键问题
  - 每个象素对应时间/年龄参数
    - 风化程度（Weathering Degree）
  - 每个风化程度对应的纹理值

难点：单幅图像 -〉时序关系

- 流形学习（**Manifold Learning**）
  - {高维数据} ➔结构信息

非线性降维

流形学习法

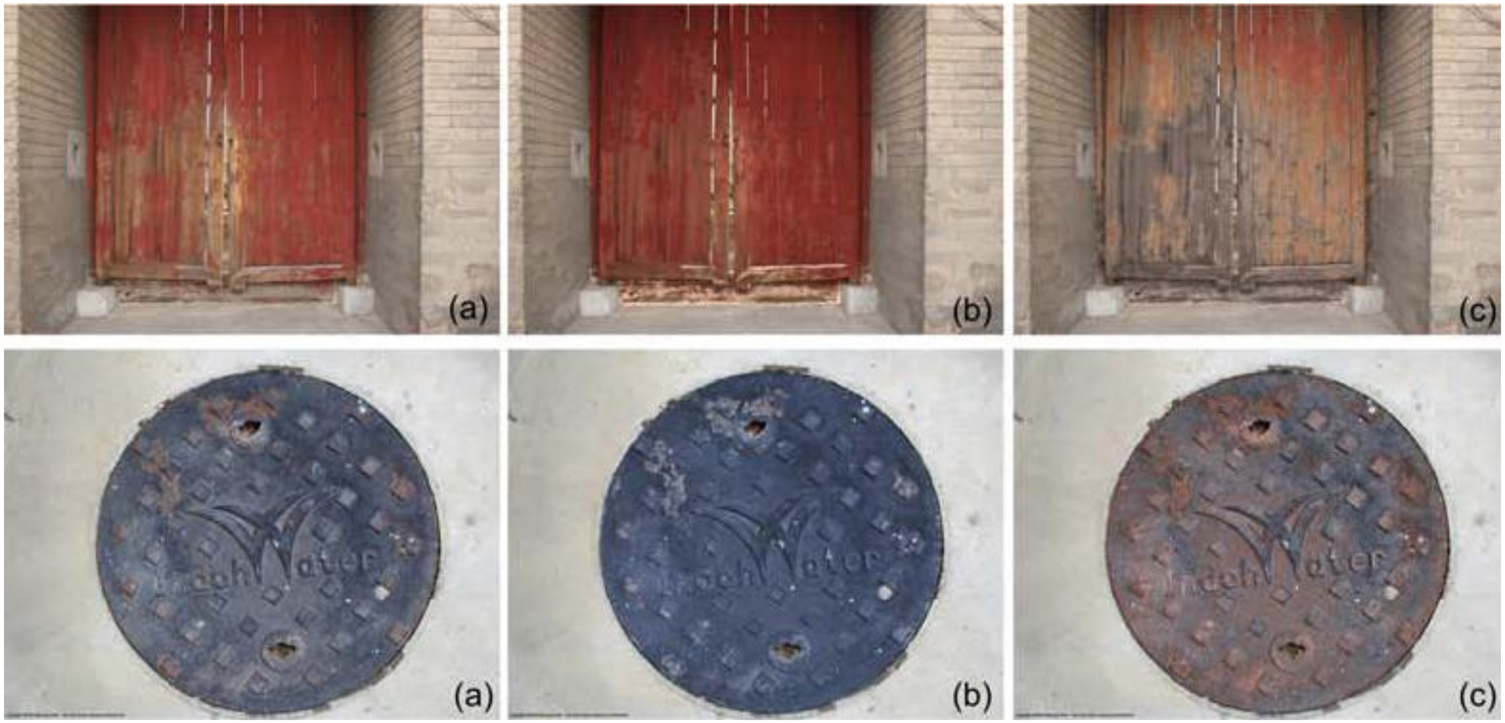


流形学习法—合成结果

- 曲面上的合成方法等
- 存储、绘制等等

流形学习法—合成结果

原图 做新 做旧



Homework

- Algorithm implementations
  - Eigenface
  - ISOMAP

- Read the ISOMAP, LLE and BoostMap papers.

- Keep on thinking:
  - How to use dimension reduction results