Spectral Methods for Dimensionality Reduction

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UCLA IPAM Tutorial, July 11-14, 2005

Dimensionality reduction

- Question

  How can we detect low dimensional structure in high dimensional data?

- Applications
  - Digital image and speech libraries
  - Neuronal population activities
  - Gene expression microarrays
  - Financial time series

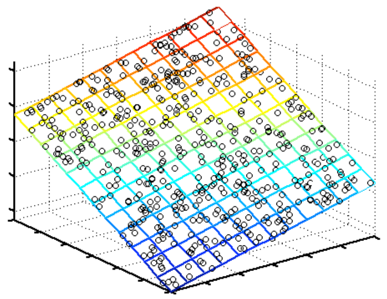
Framework

- **Data representation**

  Inputs are real-valued vectors in a high dimensional space.

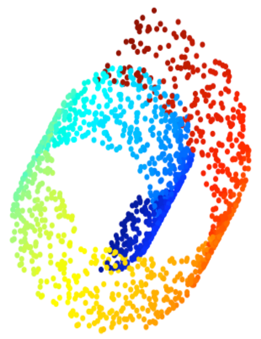
- **Linear structure**

  Does the data live in a low dimensional subspace?

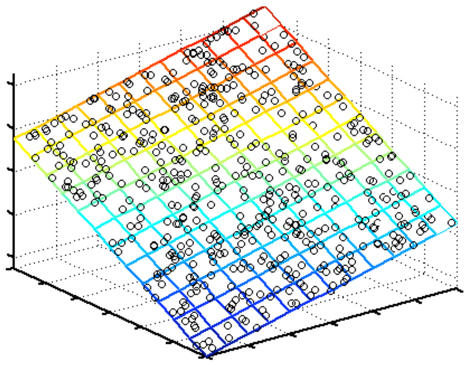


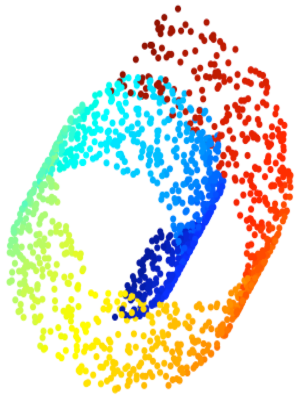
- **Nonlinear structure**

  Does the data live on a low dimensional submanifold?



Linear vs nonlinear





What computational price must we pay for nonlinear dimensionality reduction?

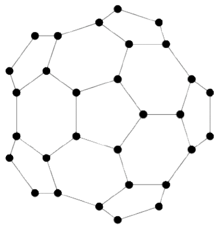
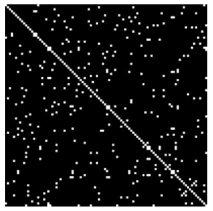
Spectral methods

- **Matrix analysis**

  Low dimensional structure is revealed by eigenvalues and eigenvectors.

- **Links to spectral graph theory**

  Matrices are derived from sparse weighted graphs.

- **Usefulness**

  Tractable methods can reveal nonlinear structure.

Notation

- **Inputs (high dimensional)**

  $\vec{x}_i \qquad {}^{D}$ with $i = 1, 2, \ldots, n$

- **Outputs (low dimensional)**

  $\vec{y}_i \qquad {}^{d}$ where $d \ll D$

- **Goals**

  Nearby points remain nearby.
  Distant points remain distant.
  (Estimate *d*.)

Manifold learning

Given high dimensional data sampled from a low dimensional submanifold, how to compute a faithful embedding?

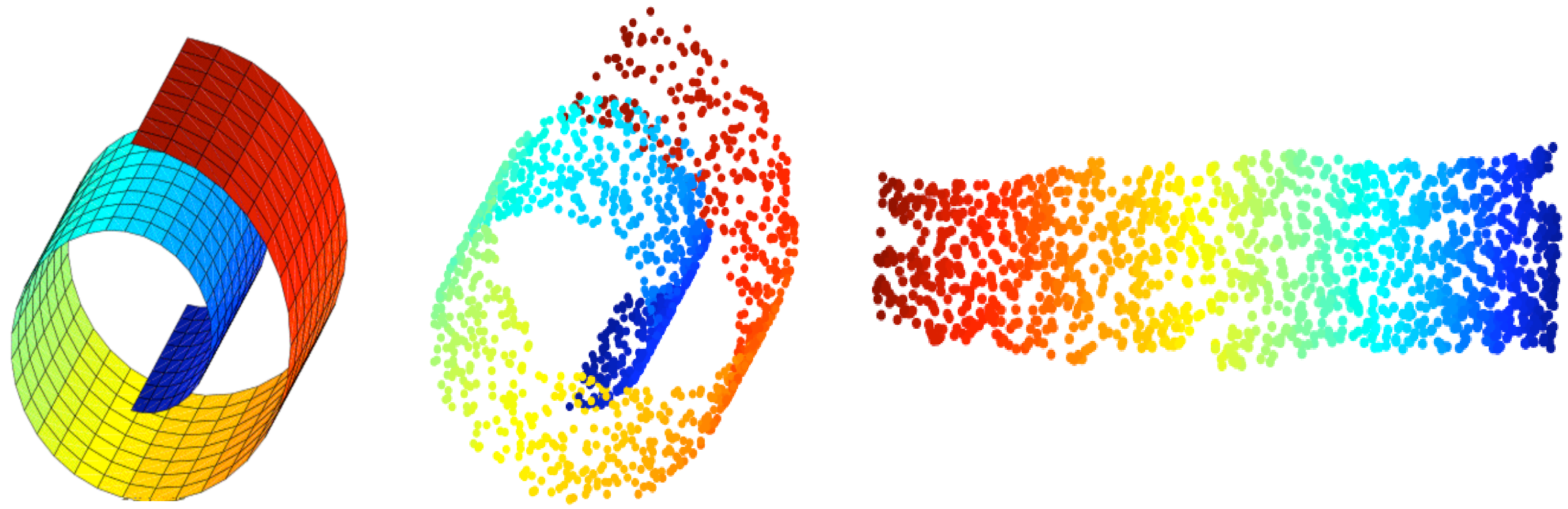
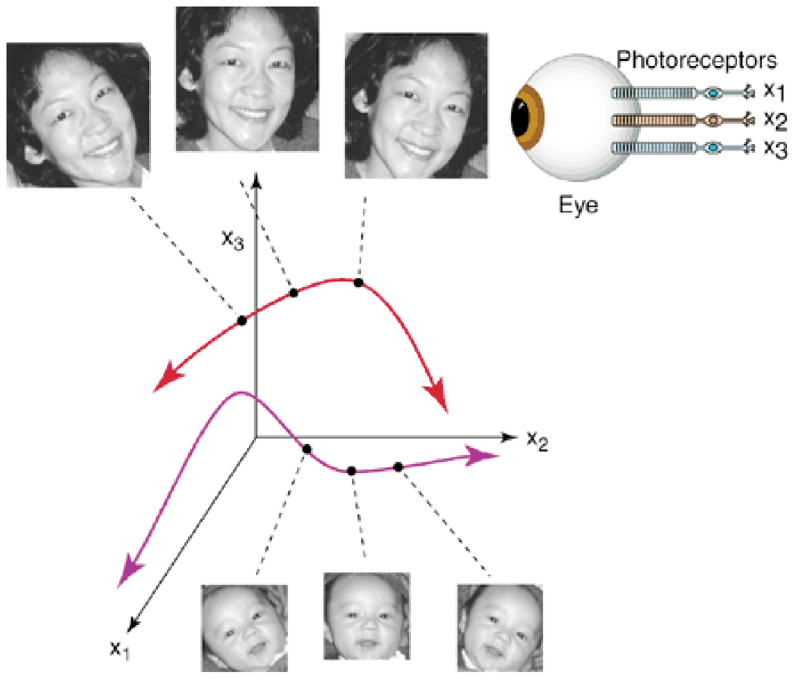
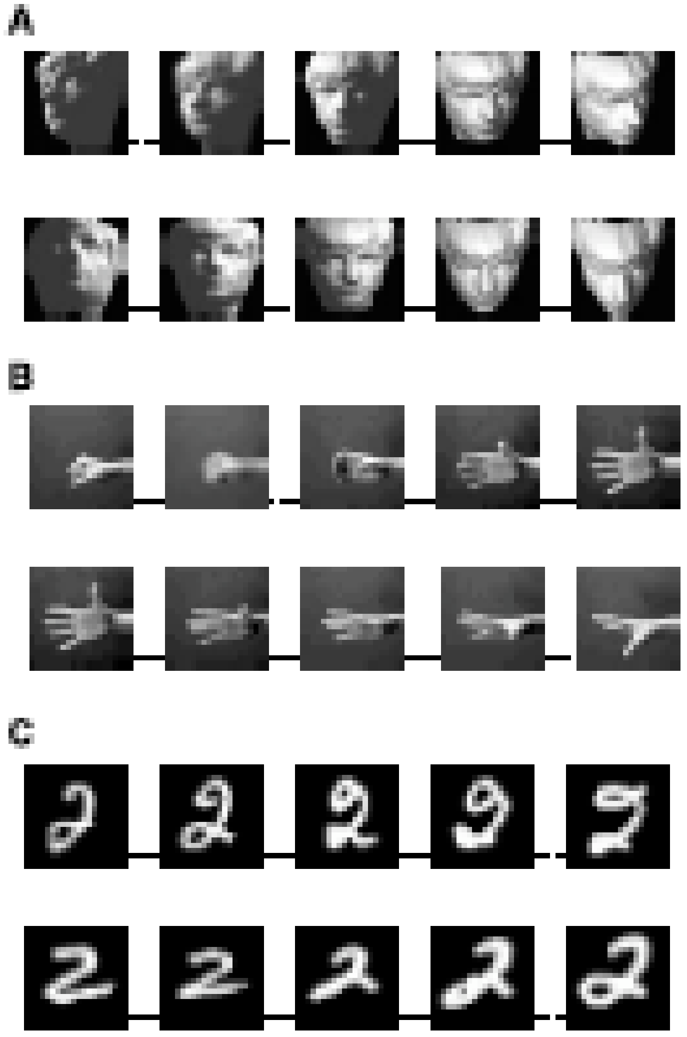


Image Manifolds





(Seung & Lee, 2000)
(Tenenbaum et al, 2000)

Outline

- Day 1 - linear, nonlinear, and graph-based methods
- Day 2 - sparse matrix methods
- Day 3 - semidefinite programming
- Day 4 - kernel methods

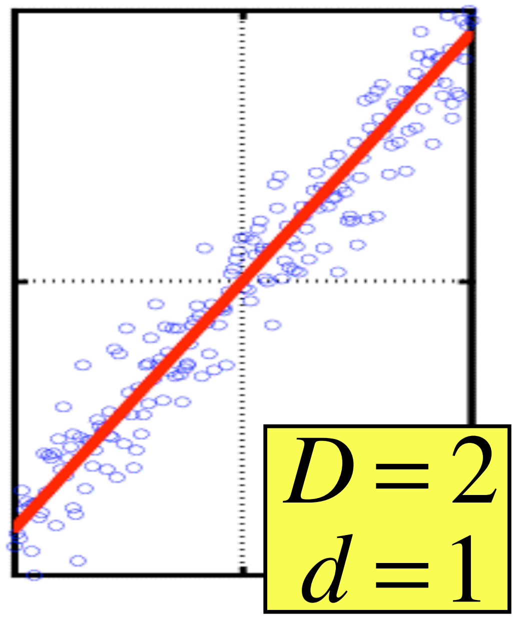
Questions for today

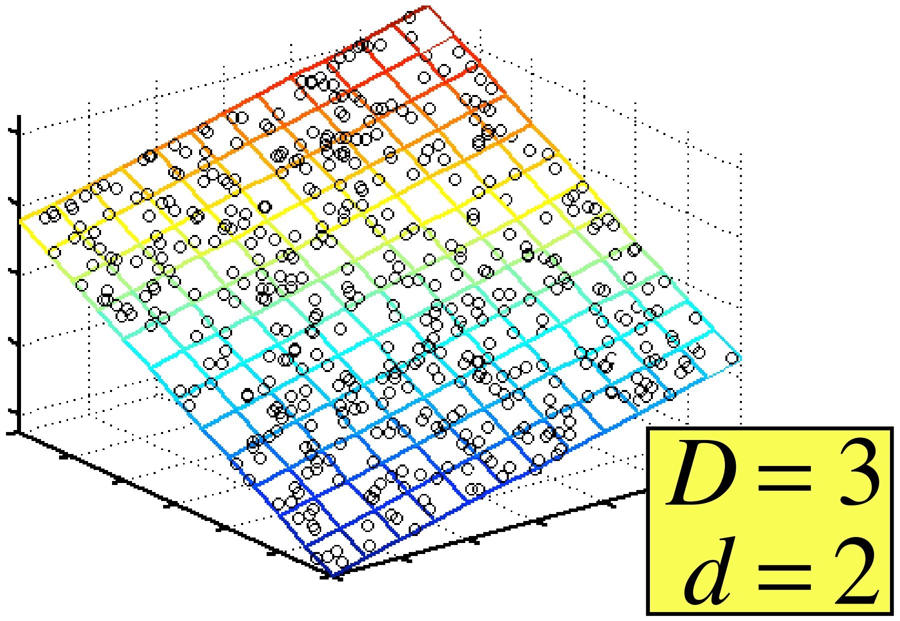
- How to detect linear structure?
  - principal components analysis
  - metric multidimensional scaling
- How (not) to generalize these methods?
  - neural network autoencoders
  - nonmetric multidimensional scaling
- How to detect nonlinear structure?
  - graphs as discretized manifolds
  - Isomap algorithm

Linear method #1

Principal Components Analysis (PCA)

Principal components analysis





Does the data mostly lie in a subspace?
If so, what is its dimensionality?

Maximum variance subspace

- **Assume inputs are centered:**

$$\underset{i}{} \vec{x}_i = \vec{0}$$

- **Project into subspace:**

$$\vec{y}_i = P\vec{x}_i \quad \text{with} \quad P^2 = P$$

- **Maximize projected variance:**

$$\mathrm{var}(\vec{y}) = \frac{1}{n} \underset{i}{} \| P\vec{x}_i \|^2$$

Matrix diagonalization

- **Covariance matrix**

$$\mathrm{var}(\vec{y}) = \ \mathrm{Tr}(PCP^{\mathrm{T}}) \ \text{ with } \ C = n^{\ 1} \ \ {}_{i} \ \ \vec{x}_i \vec{x}_i^T$$

- **Spectral decomposition**

$$C = \ {}^{D}_{=1} \ \ \vec{e} \ \vec{e}^{\mathrm{T}} \ \text{ with } \ {}_{1} \ \ \cdots \ \ {}_{D} \ \ 0$$

- **Maximum variance projection**

$$P = \ {}^{d}_{=1} \ \ \vec{e} \ \vec{e}^{\mathrm{T}}$$

Projects into subspace spanned by top d eigenvectors.

Interpreting PCA

- **Eigenvectors:**

  principal axes of maximum variance subspace.

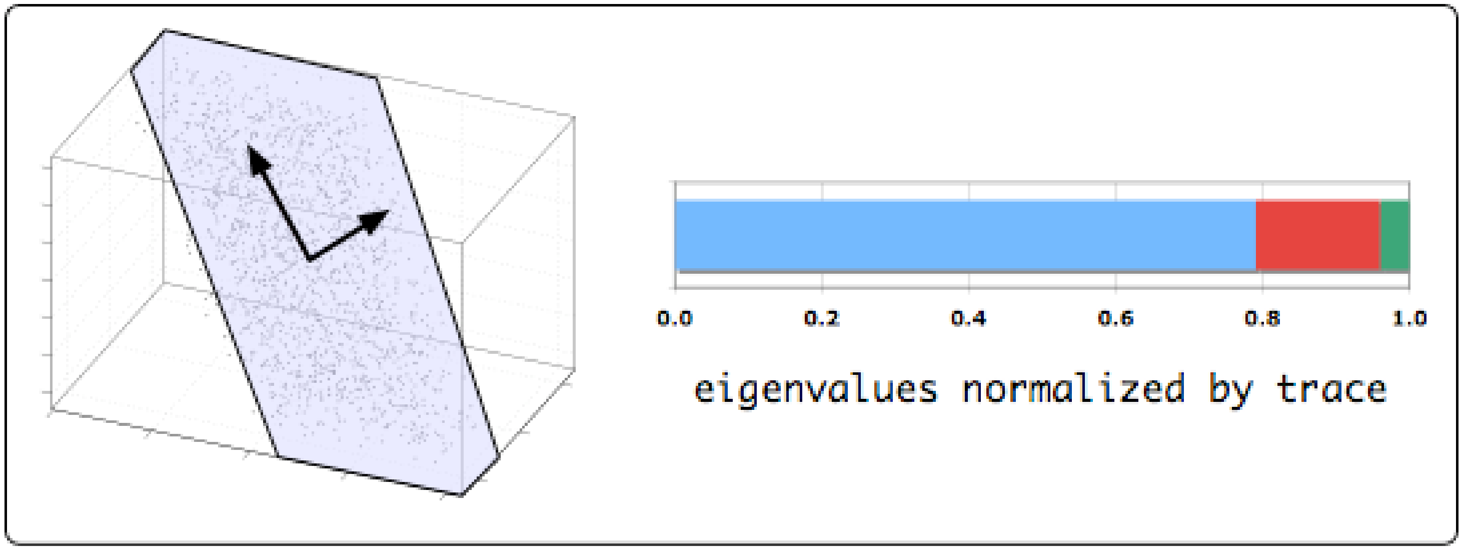
- **Eigenvalues:**

  projected variance of inputs along principle axes.

- **Estimated dimensionality:**

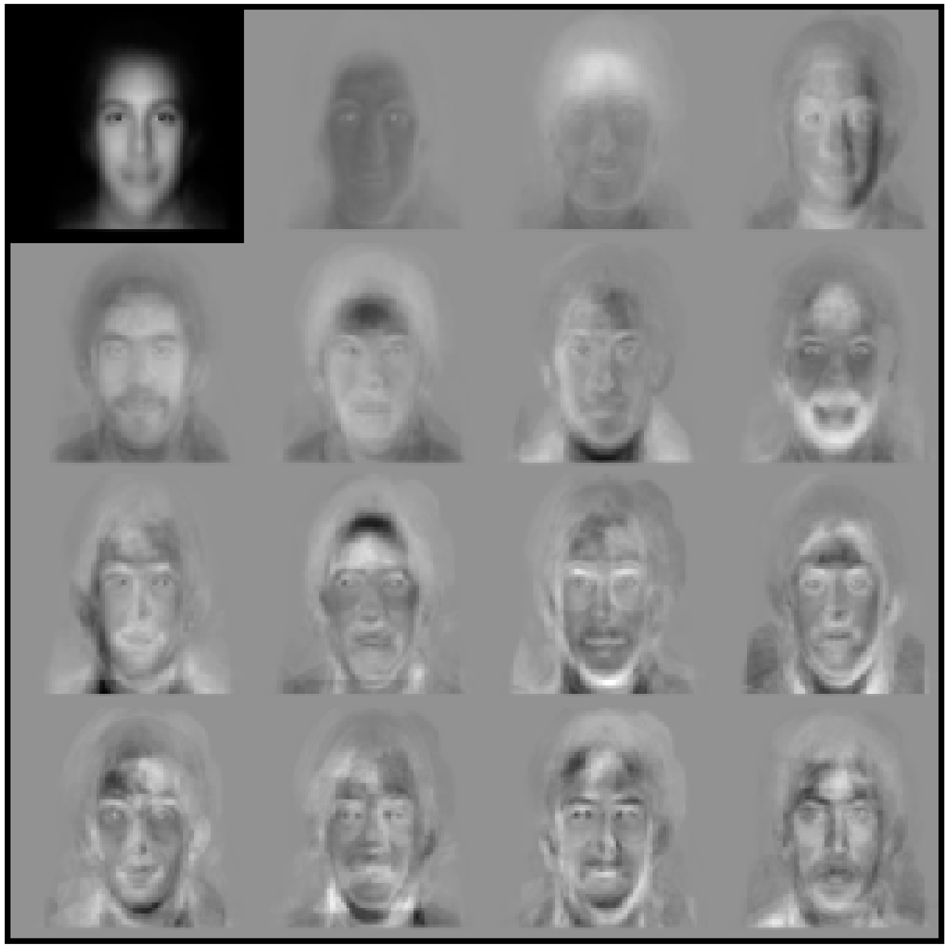
  number of significant (nonnegative) eigenvalues.

Example of PCA



Eigenvectors and eigenvalues of covariance matrix for $n=1600$ inputs in $d=3$ dimensions.

Example: faces



Eigenfaces
from 7562
images:

top left image
is linear
combination
of rest.

Sirovich & Kirby (1987)
Turk & Pentland (1991)

Another interpretation of PCA:

- **Assume inputs are centered:**

$$\vec{x}_i = \vec{0}$$

$$i$$

- **Project into subspace:**

$$\vec{y}_i = P\vec{x}_i \quad \text{with} \quad P^2 = P$$

- **Minimize reconstruction error:**

$$\mathrm{err}(\vec{y}) = n^{\;1} \qquad \|\vec{x}_i \qquad P\vec{x}_i\|^2$$

$$i$$

Equivalence

- **Minimum reconstruction error:**

$$\mathrm{err}(\vec{y}) = n^{\;1} \underset{i}{\quad} \|\vec{x}_i \quad P\vec{x}_i\|^2$$

- **Maximum variance subspace**

$$\mathrm{var}(\vec{y}) = n^{\;1} \underset{i}{\quad} \|P\vec{x}_i\|^2$$

Both models for linear dimensionality reduction yield the same solution.

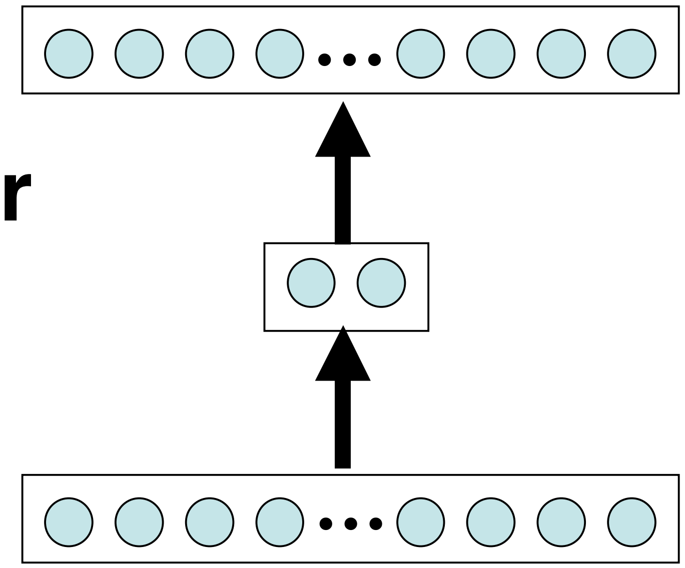
PCA as linear autoencoder

- **Network**

  Each layer implements a linear transformation.

- **Cost function**

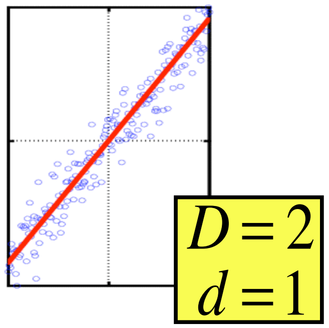
  Minimize reconstruction error through bottleneck:

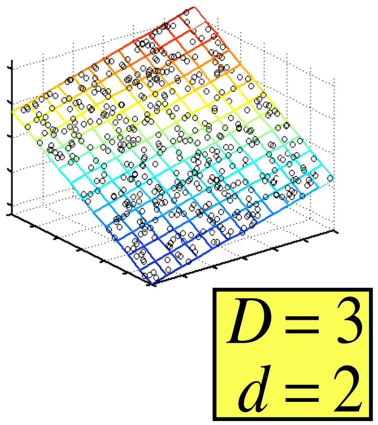


$$\mathrm{err}(P) = n^{\;1} \underset{i}{\quad} \left\| \vec{x}_i \quad P^{\mathrm{T}} P \vec{x}_i \right\|^2$$

Summary of PCA

1) **Center inputs on origin.**
2) **Compute covariance matrix.**
3) **Diagonalize.**
4) **Project.**





1) $\vec{0} = \quad {}_{i}\vec{x}_i$

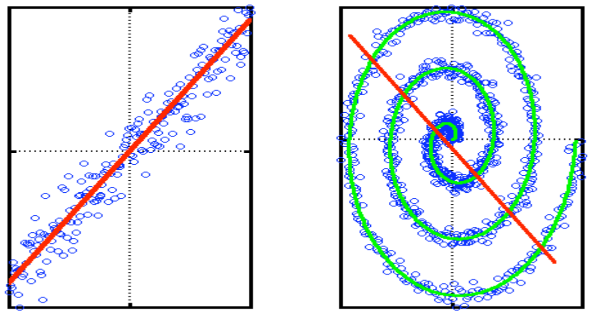
2) $C = n \quad ^{1} \quad {}_{i}\vec{x}_i\vec{x}_i^{\mathrm{T}}$

3) $C = \quad \vec{e} \ \vec{e}^{\mathrm{T}}$

4) $\vec{y}_i = P\vec{x}_i$ with $P = \quad {}_{d}\vec{e} \ \vec{e}^{\mathrm{T}}$

Properties of PCA

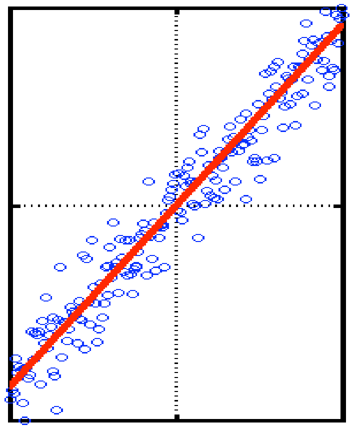
- Strengths
  - Eigenvector method
  - No tuning parameters
  - Non-iterative
  - No local optima
- Weaknesses
  - Limited to second order statistics
  - Limited to linear projections

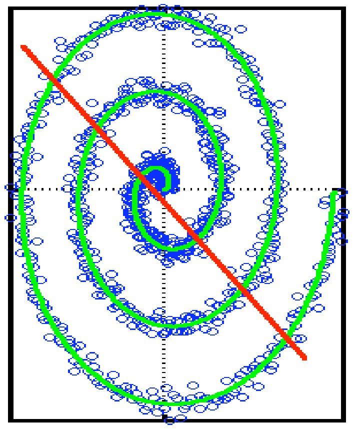


So far..

- Q: How to detect linear structure?
  A: Principal components analysis
  - Maximum variance subspace
  - Minimum reconstruction error
  - Linear network autoencoders

- Q: How (not) to generalize for manifolds?





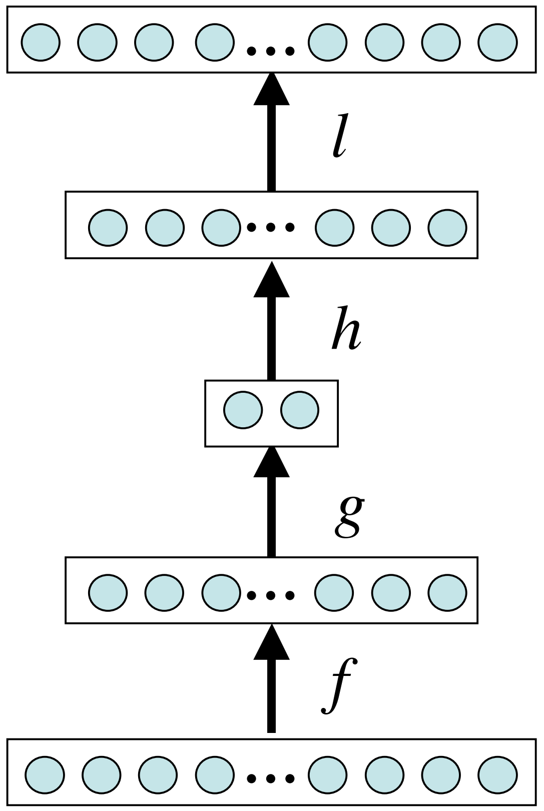
Nonlinear autoencoder

- **Neural network**

  Each layer parameterizes a nonlinear transformation.

- **Cost function**

  Minimize reconstruction error:

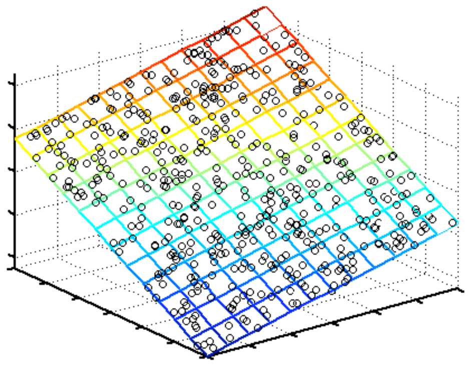


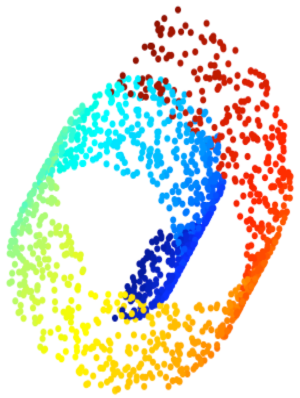
$$\mathrm{err}(W) = n^{1} \quad \underset{i}{} \left\| \vec{x}_i \quad l_W(h_W(g_W(f_W(\vec{x}_i)) \right\|^2$$

Properties of neural network

- Strengths
  - Parameterizes nonlinear mapping (in both directions).
  - Generalizes to new inputs.
- Weaknesses
  - Many unspecified choices: network size, parameterization, learning rates.
  - Highly nonlinear, iterative optimization with local minima.

Linear vs nonlinear





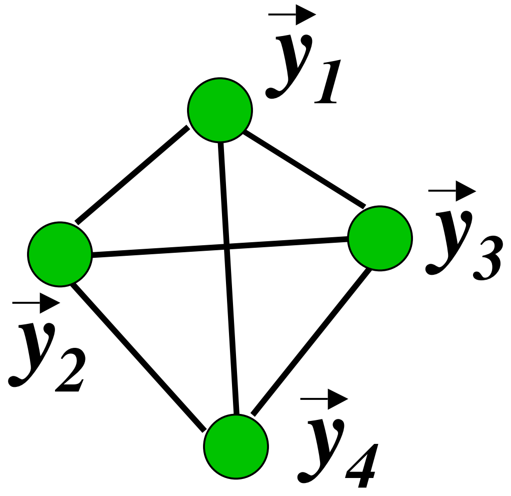
What computational price must we pay for nonlinear dimensionality reduction?

Linear method #2

Metric Multidimensional Scaling (MDS)

Multidimensional scaling

$$\begin{matrix} 0 & 12 & 13 & 14 \\ 12 & 0 & 23 & 24 \\ 13 & 23 & 0 & 34 \\ 14 & 24 & 34 & 0 \end{matrix}$$



Given $n(n\text{-}1)/2$ pairwise distances Δ_{ij}, find vectors $\vec{y}_i$ such that $\|\vec{y}_i - \vec{y}_j\| \approx \Delta_{ij}$.

Metric Multidimensional Scaling

- **Lemma**

  If Δ_{ij} denote the Euclidean distances of zero mean vectors, then the inner products are:

$$G_{ij} = \frac{1}{2} \qquad {}_{k}\Big(\quad {}^{2}_{ik} + \quad {}^{2}_{kj} \Big) \qquad {}^{2}_{ij} \qquad {}_{kl} \quad {}^{2}_{kl}$$

- **Optimization**

  Preserve dot products (proxy for distances). Choose vectors $\vec{y}_i$ to minimize:

$$\mathrm{err}(\vec{y}) = \qquad {}_{ij}\Big(G_{ij} \qquad \vec{y}_i \bullet \vec{y}_j \Big)^2$$

Matrix diagonalization

- **Gram matrix "matching"**

$$\text{err}(\vec{y}) = \quad {}_{ij}\left(G_{ij} \quad \vec{y}_i \bullet \vec{y}_j \right)^2$$

- **Spectral decomposition**

$$G = \quad \overset{n}{\underset{=1}{}} \quad \vec{v} \;\; \vec{v}^{\mathrm{T}} \;\; \text{with} \quad {}_1 \quad \cdots \quad {}_n \quad 0$$

- **Optimal approximation**

$$\boxed{y_i \quad = \sqrt{} \quad v \;\, {}_i \quad \text{for} \quad = 1,2,\ldots,d \;\; \text{with } d \quad n}$$

(scaled truncated eigenvectors)

Interpreting MDS

$$y_i = \sqrt{\quad} \; v_{\;i} \quad \text{for} \qquad = 1,2,\ldots,d \quad \text{with } d \ll n$$

- **Eigenvectors**

  Ordered, scaled, and truncated to yield low dimensional embedding.

- **Eigenvalues**

  Measure how each dimension contributes to dot products.

- **Estimated dimensionality**

  Number of significant (nonnegative) eigenvalues.

Relation to PCA

- Dual matrices

$$C \quad = n^{\ 1} \quad {}_{i}x_i \;\; x_i \quad \text{covariance matrix } (D \quad D)$$
$$G_{ij} = \vec{x}_i \bullet \vec{x}_j \qquad \text{Gram matrix} \qquad (n \quad n)$$

- Same eigenvalues

  Matrices share nonzero eigenvalues up to constant factor.

- Same results, different computation

  PCA scales as $O((n+d)D^2)$.
  MDS scales as $O((D+d)n^2)$.

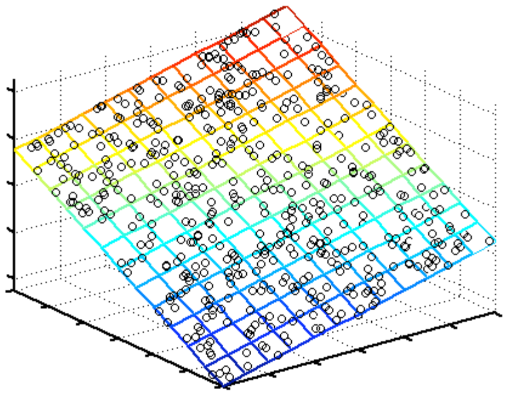
So far..

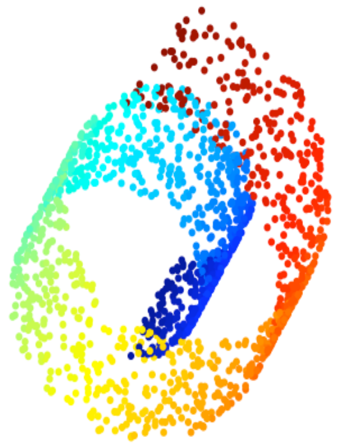
- Q: How to detect linear structure?

  A1: Principal components analysis

  A2: Metric multidimensional scaling

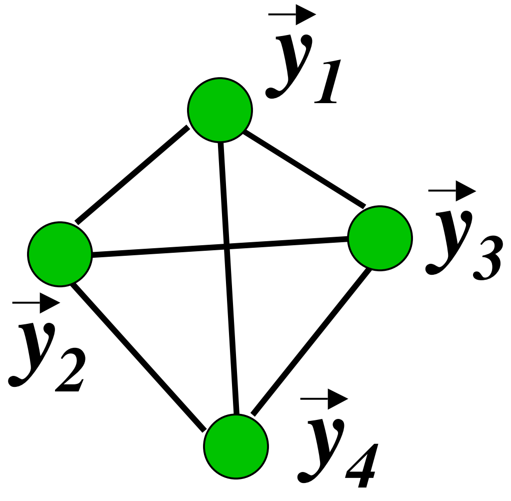
- Q: How (not) to generalize for manifolds?





Nonmetric MDS

$$\begin{matrix} 0 & 12 & 13 & 14 \\ 12 & 0 & 23 & 24 \\ 13 & 23 & 0 & 34 \\ 14 & 24 & 34 & 0 \end{matrix}$$



Transform pairwise distances: $\Delta_{ij} \longrightarrow g(\Delta_{ij})$.
Find vectors $\vec{y}_i$ such that $\|\vec{y}_i - \vec{y}_j\| \approx g(\Delta_{ij})$.

Non-Metric MDS

- **Distance transformation**

  Nonlinear, but monotonic.
  Preserves rank order of distances.

- **Optimization**

  Preserve transformed distances.
  Choose vectors $\vec{y}_i$ to minimize:

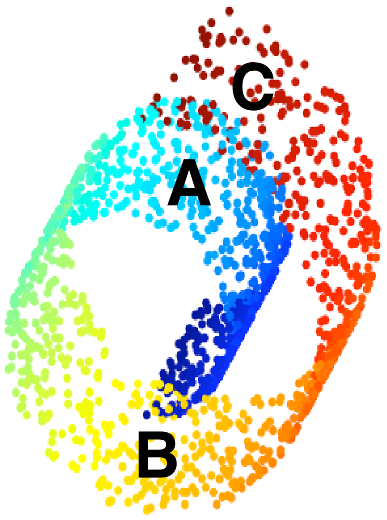
$$\boxed{\mathrm{err}(\vec{y}) = \quad {}_{ij}\Big(g(\quad {}_{ij}) \quad \|\vec{y}_i \quad \vec{y}_j\|\Big)^2}$$

Properties of non-metric MDS

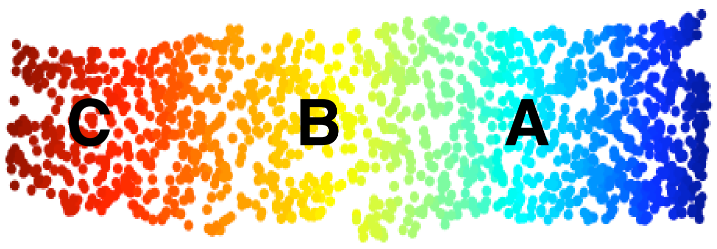
- Strengths
  - Relaxes distance constraints.
  - Yields nonlinear embeddings.
- Weaknesses
  - Highly nonlinear, iterative optimization with local minima.
  - Unclear how to choose distance transformation.

Non-metric MDS for manifolds?

Rank ordering of Euclidean distances is NOT preserved in “manifold learning”.

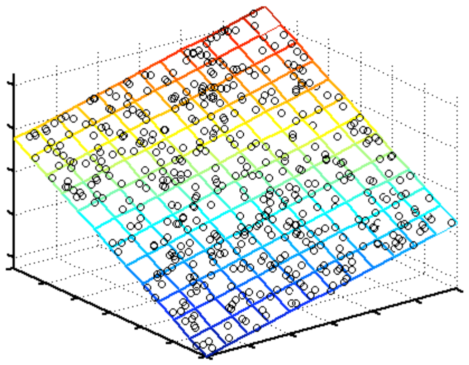


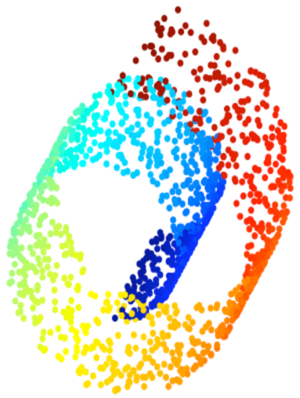
$d(A,C) < d(A,B)$



$d(A,C) > d(A,B)$

Linear vs nonlinear





What computational price must we pay for nonlinear dimensionality reduction?

Graph-based method #1

Isometric mapping of data manifolds (ISOMAP)

(Tenenbaum, de Silva, & Langford, 2000)

Dimensionality reduction

- **Inputs**

$$\vec{x}_i \qquad {}^{D} \text{ with } i = 1, 2, \ldots, n$$

- **Outputs**

$$\vec{y}_i \qquad {}^{d} \text{ where } d \ll D$$

- **Goals**

Nearby points remain nearby.
Distant points remain distant.
(Estimate *d*.)

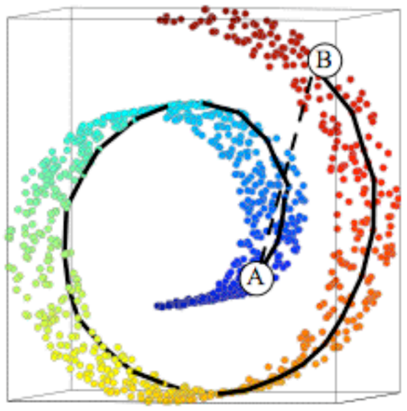
Isomap

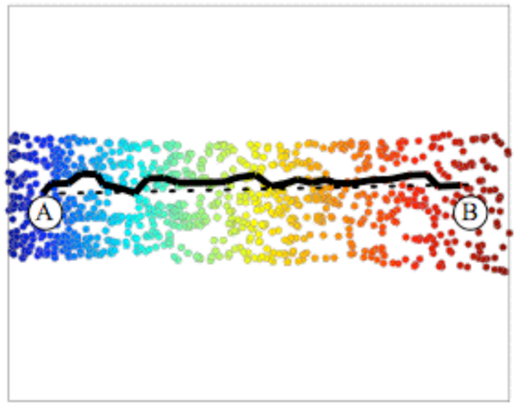
- **Key idea:**

  Preserve geodesic distances as measured along submanifold.

- **Algorithm in a nutshell:**

  Use geodesic instead of (transformed) Euclidean distances in MDS.





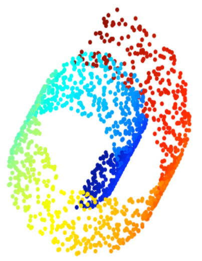
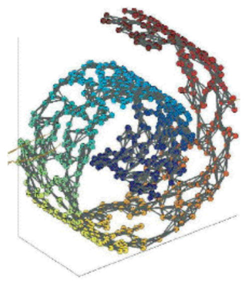
Step 1. Build adjacency graph.

- **Adjacency graph**

  Vertices represent inputs.
  Undirected edges connect neighbors.

- **Neighborhood selection**

  Many options: k-nearest neighbors, inputs within radius r, prior knowledge.

Graph is discretized approximation of submanifold.

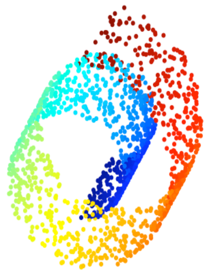
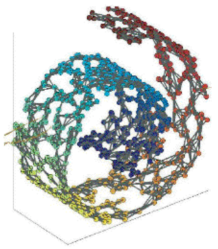
Building the graph

- **Computation**

  kNN scales naively as $O(n^2 D)$.
  Faster methods exploit data structures.

- **Assumptions**

  1) Graph is connected.
  2) Neighborhoods on graph reflect neighborhoods on manifold.

No "shortcuts" connect different arms of swiss roll.

Step 2. Estimate geodesics.

- **Dynamic programming**

  Weight edges by local distances.
  Compute shortest paths through graph.

- **Geodesic distances**

  Estimate by lengths Δ_{ij} of shortest paths:
  denser sampling = better estimates.

- **Computation**

  Djikstra's algorithm for shortest paths
  scales as $O(n^2 \log n + n^2 k)$.

Step 3. Metric MDS

- **Embedding**

  Top d eigenvectors of Gram matrix yield embedding.

- **Dimensionality**

  Number of significant eigenvalues yield estimate of dimensionality.

- **Computation**

  Top d eigenvectors can be computed in $O(n^2d)$.

Summary

- Algorithm

  1) k nearest neighbors

  2) shortest paths through graph

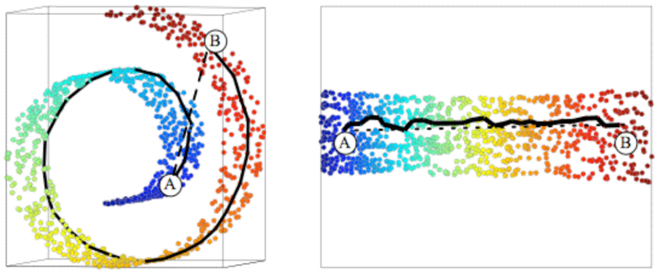
  3) MDS on geodesic distances

- Impact

  Much simpler than earlier algorithms for manifold learning. Does it work?

Examples

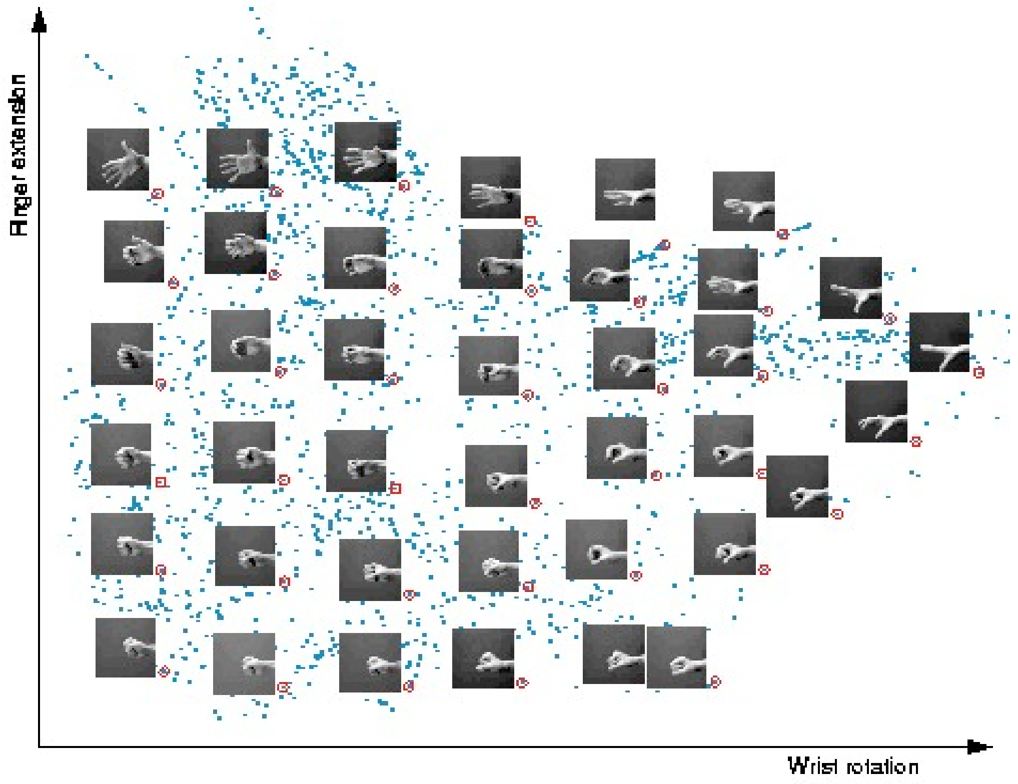
- **Swiss roll**



$n = 1024$
$k = 12$

- **Wrist images**

$n = 2000$
$k = 6$
$D = 64^2$



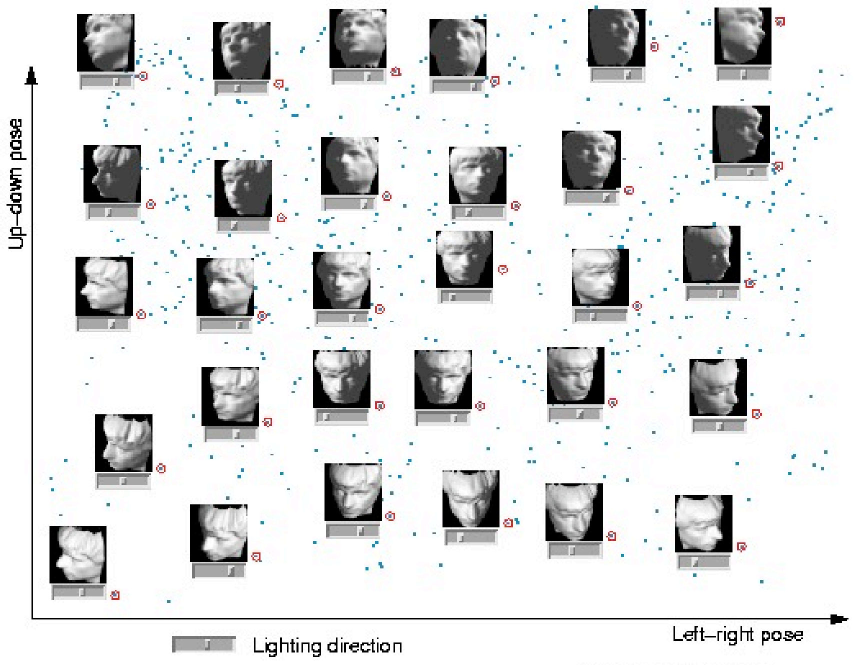
Examples

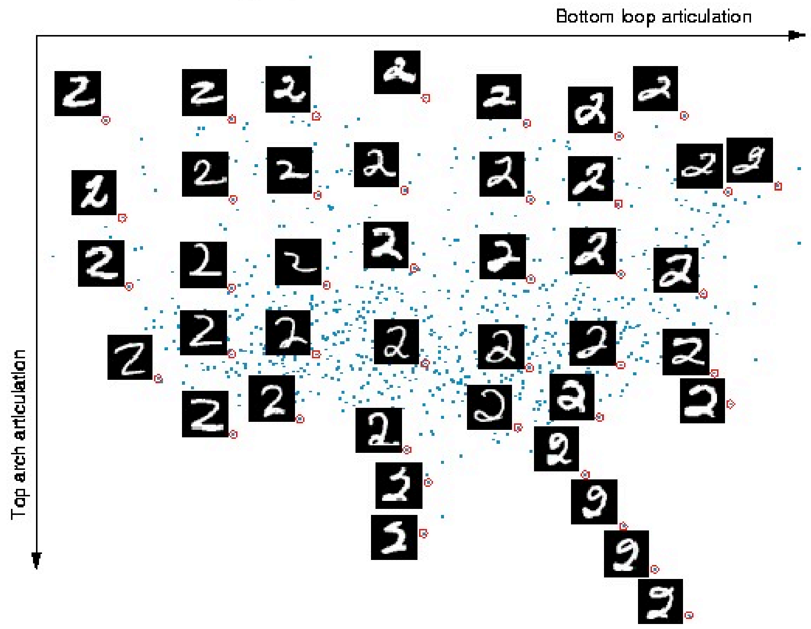
- Face images

$$\boxed{\begin{aligned} n &= 698 \\ k &= 6 \end{aligned}}$$

- Digit images

$$\boxed{\begin{aligned} n &= 1000 \\ r &= 4.2 \\ D &= 20^2 \end{aligned}}$$

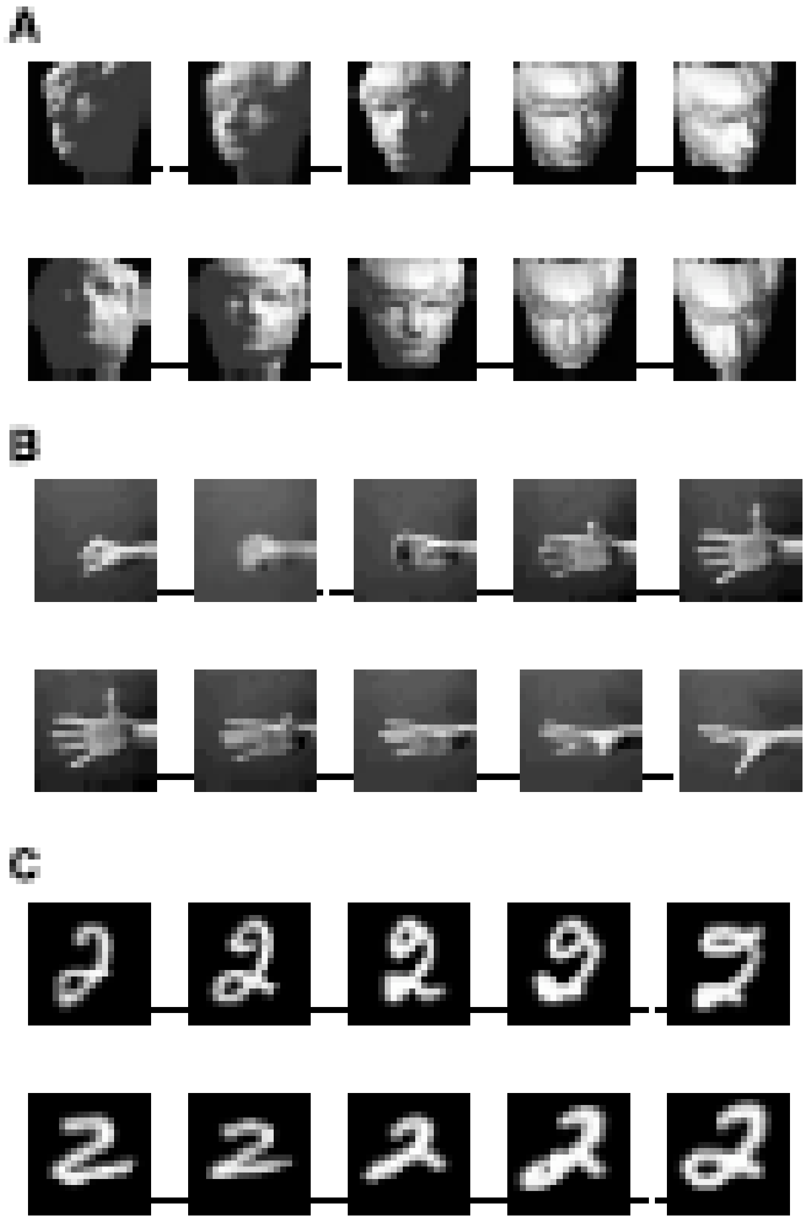




Interpolations

A. Faces
B. Wrists
C. Digits

Linear in Isomap feature space.
Nonlinear in pixel space.



Properties of Isomap

- Strengths
  - Polynomial-time optimizations
  - No local minima
  - Non-iterative (one pass thru data)
  - Non-parametric
  - Only heuristic is neighborhood size.
- Weaknesses
  - Sensitive to “shortcuts”
  - No out-of-sample extension

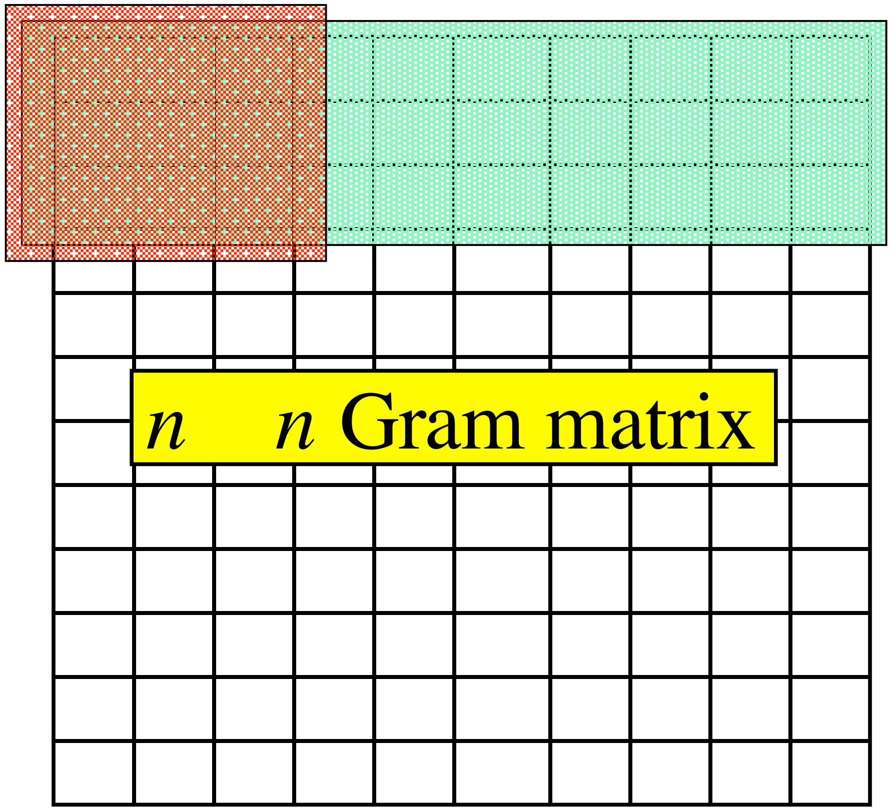
Large-scale applications

Problem:

Too expensive to compute all shortest paths and diagonalize full Gram matrix.

Solution:

Only compute shortest paths in green and diagonalize sub-matrix in red.



Landmark Isomap

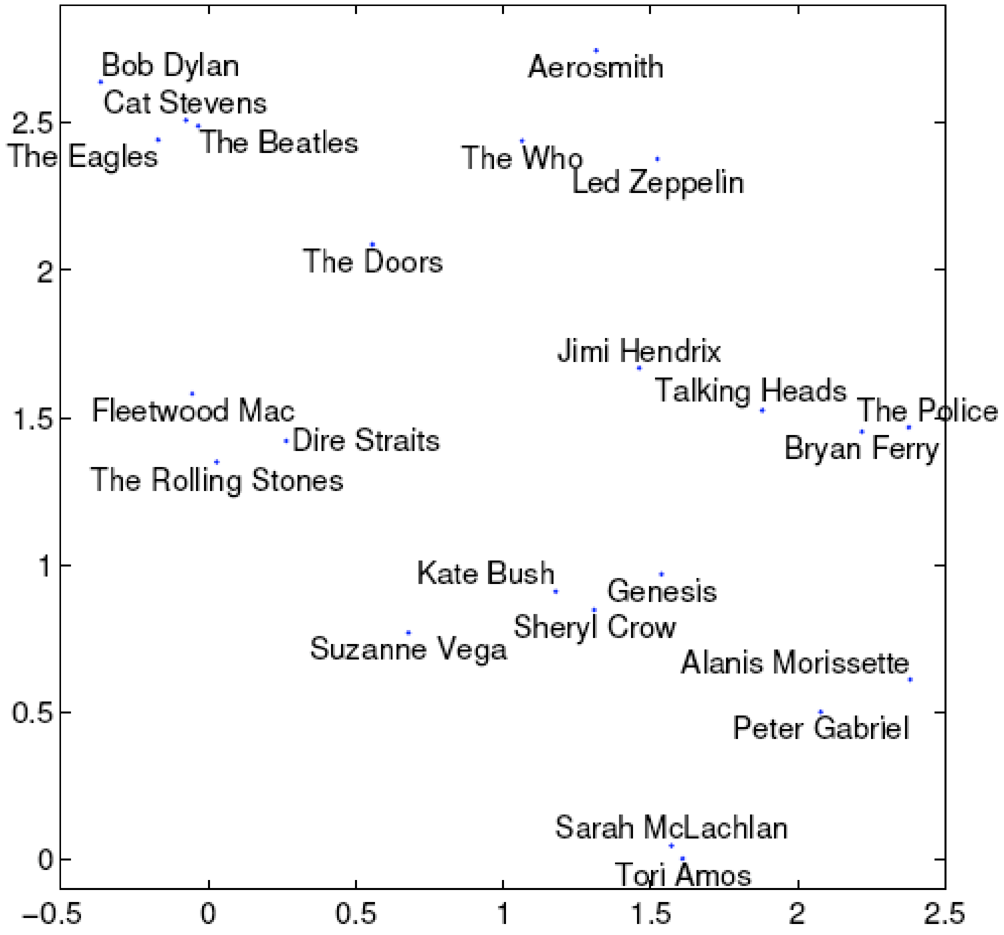
- **Approximation**
  - Identify subset of inputs as landmarks.
  - Estimate geodesics to/from landmarks.
  - Apply MDS to landmark distances.
  - Embed non-landmarks by triangulation.
  - Related to Nystrom approximation.
- **Computation**
  - Reduced by l/n for $l<n$ landmarks.
  - Reconstructs large Gram matrix from thin rectangular sub-matrix.

Example

Embedding of sparse music similarity graph

$$n = 267\text{K}$$
$$e = 3.22\text{M}$$
$$\ell = 400$$
$$= 6 \text{ minutes}$$

(Platt, 2004)



Theoretical guarantees

- Asymptotic convergence

  For data sampled from a submanifold that is isometric to a convex subset of Euclidean space, Isomap will recover the subset up to rotation & translation.

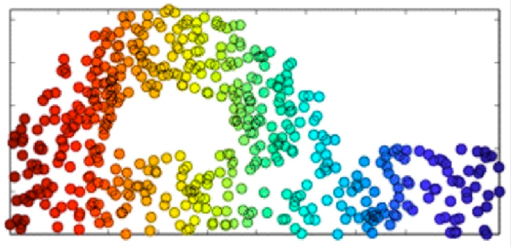
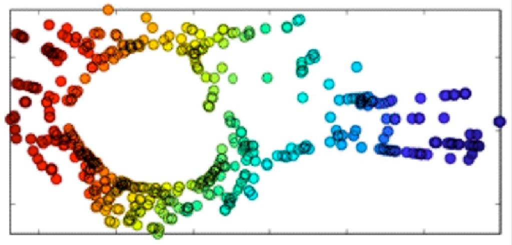
  (Tenenbaum et al; Donoho & Grimes)

- Convexity assumption

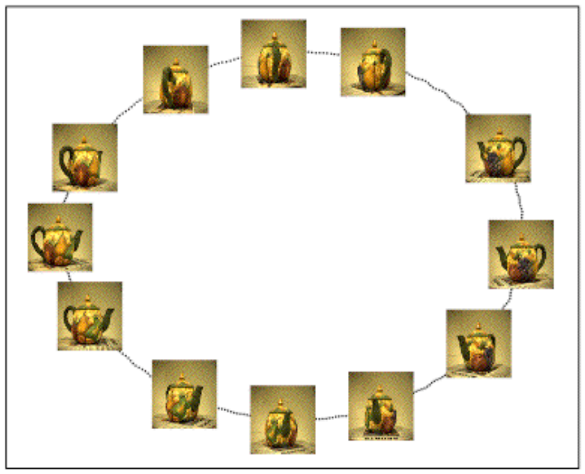
  Geodesic distances are not estimated correctly for manifolds with holes…

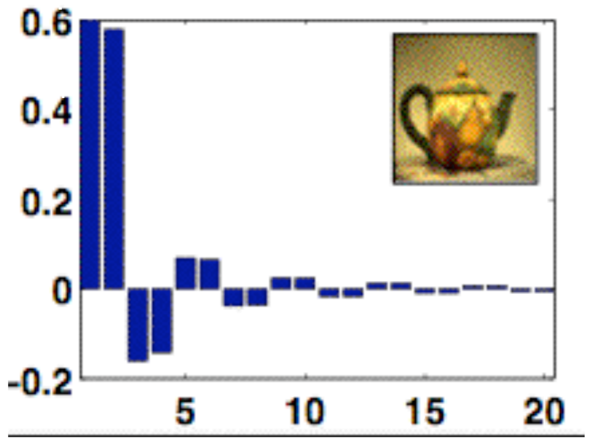
Connected but not convex

- 2d region with hole

input   Isomap

- Images of 360º rotated teapot



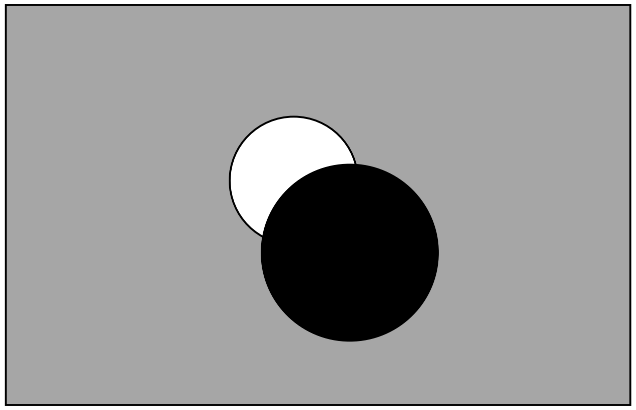


eigenvalues of Isomap

Connected but not convex

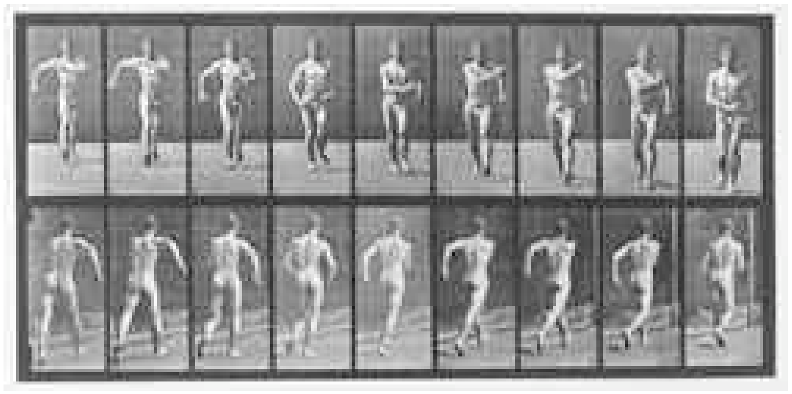
- **Occlusion**

  Images of two disks, one occluding the other.

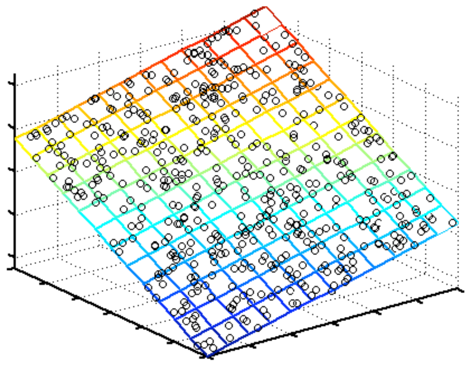


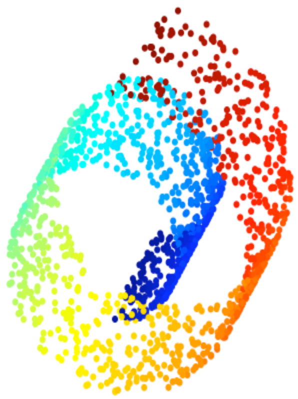
- **Locomotion**

  Images of periodic gait.



Linear vs nonlinear





What computational price must we pay for nonlinear dimensionality reduction?

Nonlinear dimensionality reduction since 2000…

These strengths and weaknesses are typical of graph-based spectral methods for dimensionality reduction.

Properties of Isomap

- Strengths
  - Polynomial-time optimizations
  - No local minima
  - Non-iterative (one pass thru data)
  - Non-parametric
  - Only heuristic is neighborhood size.
- Weaknesses
  - Sensitive to “shortcuts”
  - No out-of-sample extension

Spectral Methods

- Common framework

  1) Derive sparse graph from kNN.

  2) Derive matrix from graph weights.

  3) Derive embedding from eigenvectors.

- Varied solutions

  Algorithms differ in step 2.

  Types of optimization: shortest paths, least squares fits, semidefinite programming.

Algorithms

2000
Isomap
(Tenenbaum, de Silva, & Langford)

Locally Linear Embedding
(Roweis & Saul)

2002
Laplacian eigenmaps
(Belkin & Niyogi)

2003
Hessian LLE
(Donoho & Grimes)

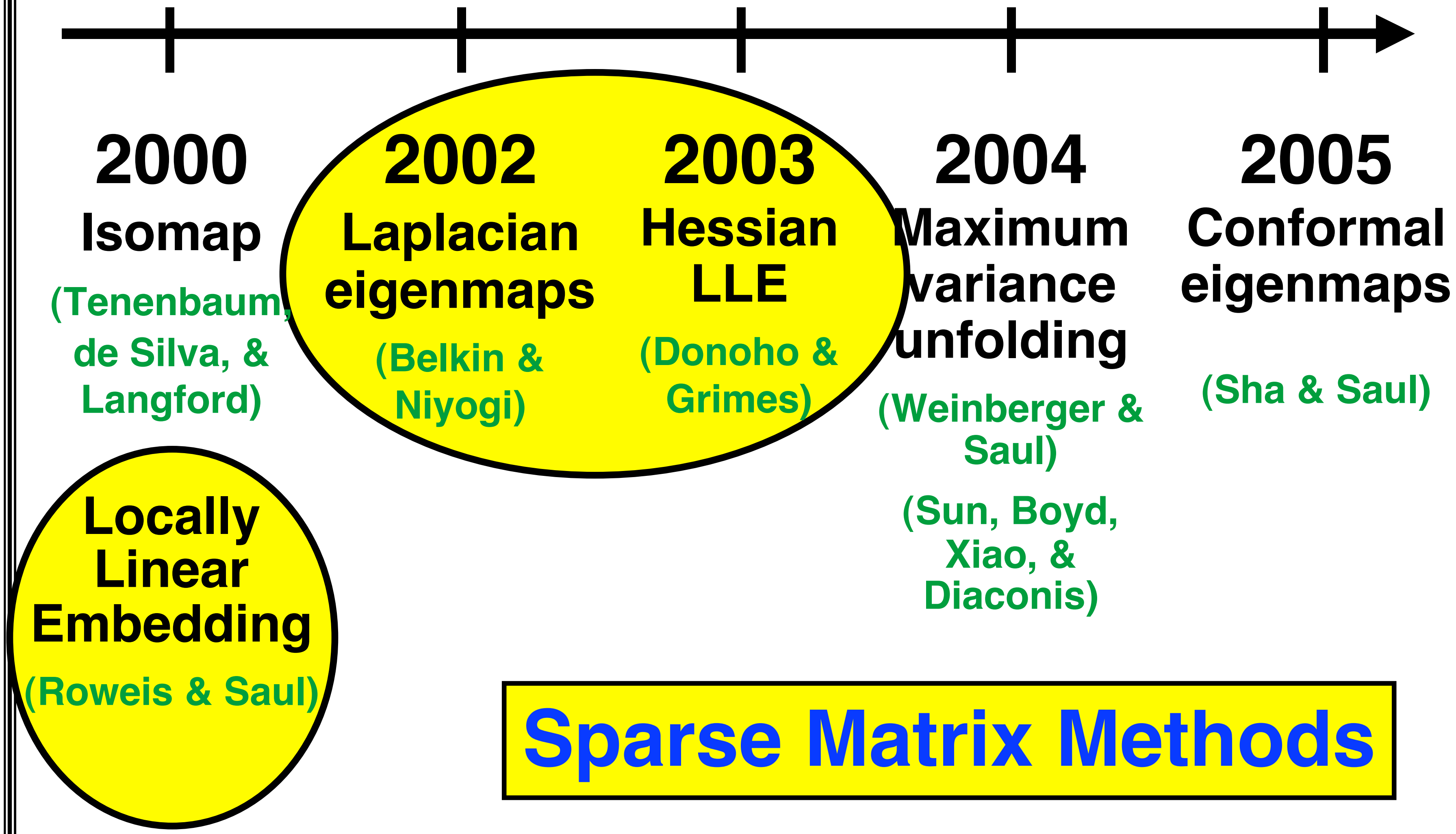
2004
Maximum variance unfolding
(Weinberger & Saul)
(Sun, Boyd, Xiao, & Diaconis)

2005
Conformal eigenmaps
(Sha & Saul)

Looking ahead

- Trade-offs
  - Sparse vs dense eigensystems?
  - Preserving distances vs angles?
  - Connected vs convex sets?
- Connections
  - Spectral graph theory
  - Convex optimization
  - Differential geometry

Tuesday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Sparse Matrix Methods

Wednesday

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Semidefinite Programming

To be continued...

See you tomorrow.