CSE 291B 2/17

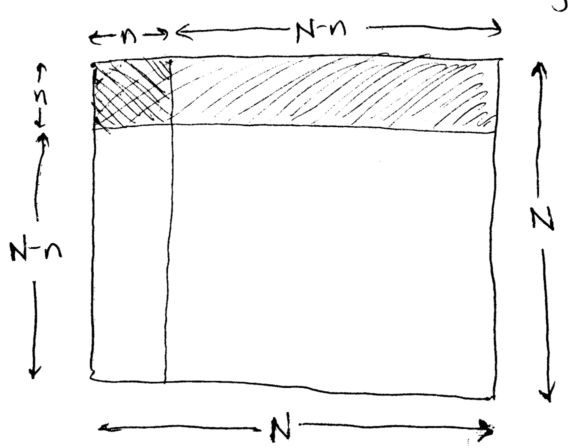
Review

- Nonlinear dimensionality reduction (NLDR)
  Given high dimensional data that lies on a low-dimensional manifold, how to compute a faithful embedding?

- Notation: inputs $\vec{x}_i \in \mathbb{R}^D$
  outputs $\vec{y}_i \in \mathbb{R}^d$ with $d \ll D$

- Isomap algorithm
  Step #1: from inputs $\vec{x}_i \in \mathbb{R}^D$, construct neighborhood graph by linking kNN $\sim O(DN^2)$
  Step #2: compute shortest paths thru graph using dynamic programming (DP) $\sim O(N^3)$
  Step #3: from graph distances, compute outputs $\vec{y}_i \in \mathbb{R}^d$ using MDS $\sim O(dN^2)$

- Scaling to large data sets
  Problem: too expensive to compute all shortest paths and eigenvectors of full gram matrix
  Solution: only compute shortest paths for $n \times (N-n)$ slab of distance matrix D_{ij}.
  only compute eigenvectors for $n \times n$ subblock of Gram matrix G_{ij}.



- Nystrom approximation

  Approximate $G = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}$ by $\tilde{G} = \left(\begin{array}{c|c} A & B \\ \hline B^T & B^T A^{-1} B \end{array}\right)$

  If size(A) ≥ rank(G) and if A is full rank, then approximation is exact.
  Why? Because rows are linearly dependent.

  In practice, G is full rank, but dominated by few large eigenvalues.

  Why? Because data is intrinsically low-dimensional.

  Approximation not exact but highly accurate.

- Timeline

2000	2002	2004
Isomap Locally linear embedding (LLE)	Laplacian eigenmaps	Maximum variance unfolding (MVU)

$\boxed{\text{Detour: semidefinite programming}}$

- Def: a semidefinite program (SDP) is a linear program with an extra constraint that a matrix whose elements are linear in the unknowns is positive semidefinite (PSD) with no negative eigenvalues.

- Ex: X is unknown matrix

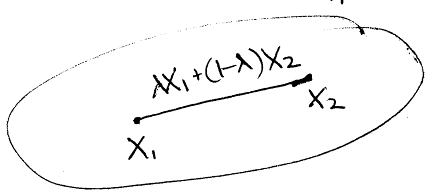
  Maximize $tr(AX)$ such that:

  (i) $tr(B_i X) \geq c_i$ for $i = 1..$ # constraints

  (ii) $X \succeq 0$ PSD constraint

- Convex optimization

  If X_1 and X_2 are both PSD,
  then so is $\lambda X_1 + (1-\lambda) X_2$ is also PSD for $\lambda \in [0,1]$.



Efficient (poly-time) algorithms exist to solve SDPs (i.e. compute global optima).

Maximum variance unfolding

- Outline
  Step #1 — compute kNN graph
  Step #2 — "unfold" graph by solving SDP
  Step #3 — apply MDS to "unfolded" graph
- Comparison to Isomap
  - same in steps #1 and #3
  - SDP vs. DP in step #2

Intuition:
To straighten a string, pull on its ends.
To flatten a sheet, pull on its four corners.
How does this idea extend to higher dimensions?

- Quadratic programming (QP)
  Maximize $\sum_i \|\vec{y}_i\|^2$ subject to:
  (i) $\|\vec{y}_i - \vec{y}_j\|^2 = \|\vec{x}_i - \vec{x}_j\|^2$ if $\vec{x}_i$ and $\vec{x}_j$ are kNN
  (ii) $\sum_i \vec{y}_i = \vec{0}$

  I.e. maximize variance of output subject to
  (i) local distance and (ii) centering constraints.
  Note: variance is bounded if kNN graph is connected.

- Inuition
  Connect kNN inputs by rigid rods.
  Pull inputs apart without breaking rods.
  Output final configuration.
- Alternative formulations of distance constraints
  $\|\vec{y}_i - \vec{y}_j\|^2 \leq \|\vec{x}_i - \vec{x}_j\|^2$ replace rods by strings
  $\|\vec{y}_i - \vec{y}_j\|^2 \approx \|\vec{x}_i - \vec{x}_j\|^2$ replace rods by springs
- QP is hard to solve
  Why? Maximizing (not minimizing) variance.
  Also: $\|\vec{y}_i - \vec{y}_j\|^2 = \|\vec{x}_i - \vec{x}_j\|^2$ not convex.

- Change of variables
  - Gram matrix $K_{ij} = \vec{y}_i \cdot \vec{y}_j$ determines outputs up to global rotation.
  - Replacing $\vec{y}_i \cdot \vec{y}_j$ by K_{ij}:

    Variance $\sum_i \|\vec{y}_i\|^2 = \sum_i K_{ii} = \mathrm{tr}(K)$

    this is a minus

    Distances $\|\vec{y}_i - \vec{y}_j\|^2 = \|\vec{y}_i\|^2 + \|\vec{y}_j\|^2 - 2\,\vec{y}_i \cdot \vec{y}_j = K_{ii} + K_{jj} - 2K_{ij}$

    Centering: $\sum_i \vec{y}_i = \vec{0} \longrightarrow \|(\sum_i \vec{y}_i)\|^2 = 0 \longrightarrow \sum_{ij} \vec{y}_i \cdot \vec{y}_j = \sum_{ij} K_{ij} = 0$

- Relax QP to SDP

  Maximize $\mathrm{tr}(K)$ subject to:

  (i) $K_{ii} + K_{jj} - 2K_{ij} = \|\vec{x}_i - \vec{x}_j\|^2$ if $\vec{x}_i$ and $\vec{x}_j$ are kNN

  (ii) $\sum_{ij} K_{ij} = 0$

  (iii) $K \succeq 0$ (PSD)

  Constraint (iii) relaxing the implicit rank constraint $\vec{y}_i \in \mathbb{R}^d$ in QP.

- MVU versus PCA

  PCA maximizes variance of linear projection.

  MVU maximizes variance of nonlinear (but locally distance-preserving) projections.

- MVU versus Isomap
- Similarities
  - motivated by isometry
  - based on constructing Gram matrix
  - eigenvalues reveal dimensionality
- Differences
  - SDP versus DP
  - finite vs. asymptotic guarantees
  - handling of manifolds with "holes"

- Scaling

  SDP scales at least as $O(n^3 + c^3)$ where

  $n =$ size of matrix

  $c =$ # constraints

  Naive scaling for MVU is $O(k^3 N^3)$ for N examples and kNN.

  How to improve?