Graph Laplacian Regularization for Large-Scale Semidefinite Programming

> Kilian Weinberger et al. NIPS 2006

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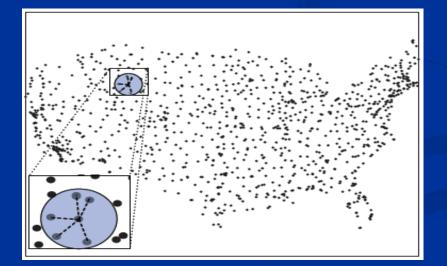
Introduction

Problem

- discovery of low dimensional representations of highdimensional data
- in many cases, local proximity measurements also available
- e.g. computer vision, sensor localization
- Current Approach
 - semidefinite programs (SDPs) convex optimization
 - Disadvantage: it doesn't scale well for large inputs
 - Paper Contribution
 - method for solving very large problems of the above type
 - much smaller/faster SDPs than those previously studied

Sensor localization

- Determine the 2D position of the sensors based on estimates of local distances between neighboring sensors
 - sensors i, j neighbors iff sufficiently close to estimate their pairwise distance via limited-range radio transmission
- Input:
 - n sensors
 - d_{ii}: estimate of local distance between neighboring sensors i,j
- Output:
 - $x_1, x_2, ..., x_n \in \mathbb{R}^2$: planar coordinates of sensors



Work so far...

Minimize sum-of-squares loss function

$$\min_{\vec{x}_1,...,\vec{x}_n} \sum_{i \sim j} \left(\|\vec{x}_i - \vec{x}_j\|^2 - d_{ij}^2 \right)^2 \tag{1}$$

Centering constraint (assuming no sensor location is known in advance)

$$\left\|\sum_{i} \vec{x}_{i}\right\|^{2} = 0 \tag{2}$$

Optimization in (1) non convex
→ Likely to be trapped in local minima !

Convex Optimization

Convex function

- a real-valued function f defined on a domain C that for any two points x and y in C and any t in [0,1],
- $f(tx + (1-t)y) \le tf(x) + (1-t)f(y)$

Convex optimization

Standard form is the usual and most intuitive form of describing a convex optimization problem. It consists of the following three parts:

- A convex function $f_0(x):\mathbb{R}^n o \mathbb{R}$ to be minimized over the variable x
- = Inequality constraints of the form $\,f_i(x)\,\leq 0$, where the functions $\,f_i\,$ are convex
- Equality constraints of the form h_i(x) = 0, where the functions h_i are affine. In practice, the terminology "linear" and "affine" are generally equivalent and most often expressed in the form Ax = b, where A is a matrix and b is a vector.

A convex optimization problem is thus written as

minimize
$$f_0(x)$$
 subject to
 $f_i(x) \le 0, \quad i = 1, \dots, m$
 $h_i(x) = 0, \quad i = 1, \dots, p$

Solution to convexity

Define n x n inner-product matrix X

 $\bullet X_{ij} = X_i \cdot X_j$

Get convex optimization by relaxing the constraint that sensor locations x_i lie in the R² plane

Minimize:
$$\sum_{i \sim j} \left(\mathbf{X}_{ii} - 2\mathbf{X}_{ij} + \mathbf{X}_{jj} - d_{ij}^2 \right)^2$$

subject to: (i)
$$\sum_{ij} \mathbf{X}_{ij} = 0 \quad \text{and} \quad \text{(ii) } \mathbf{X} \succeq 0.$$
 (3)

x_i vectors will lie in a subspace with dimension equal to the rank of the solution X

Project x_i s into their 2D subspace of maximum variance to get planar coordinates
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Maximum Variance Unfolding (MVU)

- The higher the rank of X, the greater the information loss after projection
- Add extra term to the loss function to favor solutions with high variance (or high trace)

Maximize:
$$\operatorname{tr}(\mathbf{X}) - \nu \sum_{i \sim j} \left(\mathbf{X}_{ii} - 2\mathbf{X}_{ij} + \mathbf{X}_{jj} - d_{ij}^2 \right)^2$$

subject to: (i) $\sum_{ij} \mathbf{X}_{ij} = 0$ and (ii) $\mathbf{X} \succeq 0$.

- trace of square matrix X (tr(X)): sum of the elements on X's main diagonal
- parameter v > 0 balances the trade-off between maximizing variance and preserving local distances (maximum variance unfolding - MVU)

(4)

Matrix factorization (1/2)

- G : neighborhood graph defined by the sensor network
- Assume location of sensors is a function defined over the nodes of G
- Functions on a graph can be approximated using eigenvectors of graph's Laplacian matrix as basis functions (spectral graph theory) $\frac{(\deg(w))}{(\deg(w))} = i \int_{-\infty}^{\infty} \frac{1}{2\pi} dx$

graph Laplacian I:
$$l_{i,j} := \begin{cases} \deg(v_i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } v_i \text{ adjacent } v_j \\ 0 & \text{otherwise} \end{cases}$$

- eigenvectors of graph Laplacian matrix ordered by smoothness
- Approximate sensors' locations using the m bottom eigenvectors of the Laplacian matrix of G
 - $x_i \approx \Sigma_{\alpha=1}^m Q_{i\alpha} y_{\alpha}$
 - Q : n x m matrix with the m bottom eigenvectors of Laplacian matrix (precomputed)
 - y_{α} : m x 1 vector , $\alpha = 1, ..., m$ (unknown)

Matrix factorization (2/2)

Define m x m inner-product matrix Y

 $\bullet Y_{\alpha\beta} = y_{\alpha} \cdot y_{\beta}$

- Factorize matrix X
 - $X \approx QYQ^T$
- Get equivalent optimization
 - tr(Y) = tr(X), since Q stores mutually orthogonal eigenvectors
 - QYQ^T satisfies centering constraint (uniform eigenvector not included)

 $\begin{array}{ll} \text{Maximize:} & \operatorname{tr}(\mathbf{Y}) - \nu \sum_{i \sim j} \left[(\mathbf{Q} \mathbf{Y} \mathbf{Q}^{\top})_{ii} - 2 (\mathbf{Q} \mathbf{Y} \mathbf{Q}^{\top})_{ij} + (\mathbf{Q} \mathbf{Y} \mathbf{Q}^{\top})_{jj} - d_{ij}^2 \right]^2 \\ \text{subject to:} & \mathbf{Y} \succeq 0 \end{array}$

(5)

Instead of the n x n matrix X, optimization is solved for the much smaller m x m matrix Y !

Formulation as SDP

- Approach for large input problems:
 - cast the required optimization as SDP over small matrices with few constraints
- Rewrite the previous formula as an SDP in standard form
 - \mathbf{e}^{m^2} : vector obtained by concatenating all the columns of Y
 - Ac m² x m² : positive semidefinite matrix collecting all the quadratic coefficients in the objective function
 - be ^{m2}: vector collecting all the linear coefficients in the objective function
 - I : lower bound on the quadratic piece of the objective function
 - Use Schur's lemma to express this bound as a linear matrix inequality

Maximize:
$$b^{\top} \mathcal{Y} - \ell$$
subject to:(i) $\mathbf{Y} \succeq 0$ and(ii) $\begin{bmatrix} \mathbf{I} & \mathbf{A}^{\frac{1}{2}} \mathcal{Y} \\ (\mathbf{A}^{\frac{1}{2}} \mathcal{Y})^{\top} & \ell \end{bmatrix} \succeq 0.$

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(6)

Formulation as SDP

- Approach for large input problems:
 - cast the required optimization as SDP over small matrices with few constraints

$$\begin{array}{ll} \mathbf{Maximize:} & b^{\top} \mathcal{Y} - \ell \\ \mathbf{subject \ to:} & (\mathbf{i}) \ \mathbf{Y} \succeq 0 & \mbox{ and } & (\mathbf{ii}) \left[\begin{array}{cc} \mathbf{I} & \mathbf{A}^{\frac{1}{2}} \mathcal{Y} \\ (\mathbf{A}^{\frac{1}{2}} \mathcal{Y})^{\top} & \ell \end{array} \right] \succeq 0. \end{array}$$

- Unknown variables: m(m+1)/2 elements of Y and scalar
- Constraints: positive semidefinite constraint on Y and linear matrix inequality of size m² x m²
- **The complexity of the SDP does not depend on the** 3/21/**number of nodes (n) or edges in the network**!

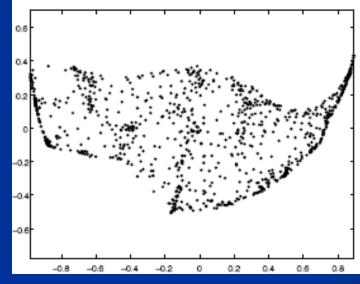
Gradient-based improvement

2-step process (optional):

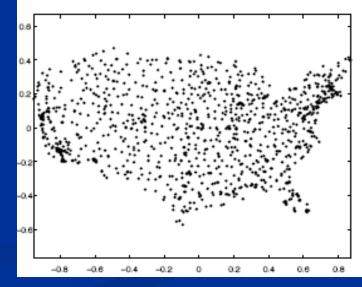
- Starting from the m-dimensional solution of eq. (6), use conjugate gradient methods to maximize the objective function in eq. (4)
- Project the results from the previous step into the R² plane and use conjugate gradient methods to minimize the loss function in eq. (1)
 - conjugate gradient method: iterative method for minimizing a quadratic function where its Hessian matrix (matrix of second partial derivatives) is positive definite

Results (1/2)

- n = 1055 largest cities in continental US
- local distances up to 18 neighbors within radius r = 0.09
- Iocal measurements corrupted by 10% Gaussian noise over the true local distance
- m = 10 bottom eigenvectors of graph Laplacian



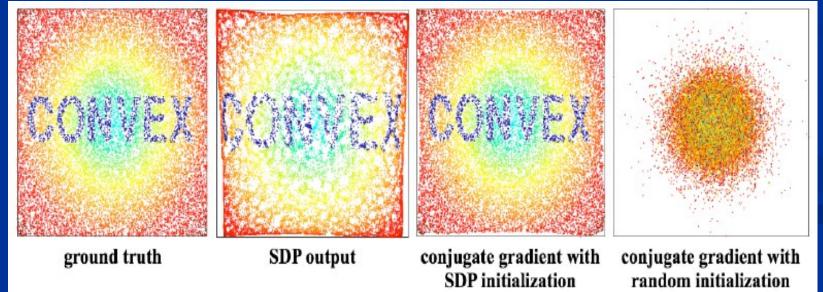
Result from SDP in $(9) \sim 4s$ 3/21/2007



Result after conjugate gradient descent

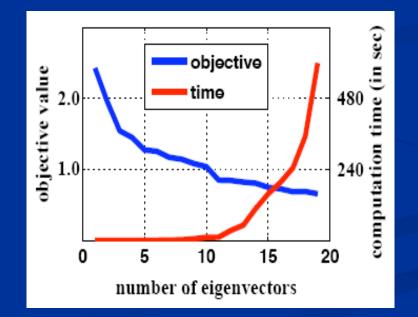
Results (2/2)

- n = 20,000 uniformly sampled points inside the unit square
- local distances up to 20 other nodes within radius r = 0.06
- m = 10 bottom eigenvectors of graph Laplacian
- 19s to construct and solve the SDP
- **52s for 100 iterations in conjugate gradient descent**



Results (3/3)

loss function in eq. (1) vs. number of eigenvectors
computation time vs. number of eigenvectors
"sweet spot" around m ≈ 10 eigenvectors



FastMVU on Robotics

Control of a robot using sparse user input
 e.g. 2D mouse position

Robot localization

the robot's location is inferred from the high dimensional description of its state in terms of sensorimotor input

Conclusion

- Approach for inferring low dimensional representations from local distance constraints using MVU
- Use of matrix factorization computed from the bottom eigenvectors of the graph Laplacian
 Local search methods can refine solution
 Suitable for large input; its complexity does not depend on the input!