Convex Optimization

Geometrical and Approximation Problems

- norm approximation
- least-norm problems
- regularized approximation
- robust approximation

minimize ||Ax - b||

 $(A \in \mathbf{R}^{m \times n} \text{ with } m \ge n, \|\cdot\| \text{ is a norm on } \mathbf{R}^m)$

interpretations of solution $x^* = \operatorname{argmin}_x \|Ax - b\|$:

- **geometric**: Ax^* is point in $\mathcal{R}(A)$ closest to b
- **estimation**: linear measurement model

y = Ax + v

y are measurements, x is unknown, v is measurement error

given y = b, best guess of x is x^*

optimal design: x are design variables (input), Ax is result (output)

 x^{\star} is design that best approximates desired result b

examples

• least-squares approximation $(\| \cdot \|_2)$: solution satisfies normal equations

$$A^T A x = A^T b$$

 $(x^{\star} = (A^T A)^{-1} A^T b \text{ if } \operatorname{\mathbf{Rank}} A = n)$

• Chebyshev approximation $(\|\cdot\|_{\infty})$: can be solved as an LP

minimize
$$t$$

subject to $-t\mathbf{1} \preceq Ax - b \preceq t\mathbf{1}$

• sum of absolute residuals approximation $(\|\cdot\|_1)$: can be solved as an LP

$$\begin{array}{ll} \text{minimize} & \mathbf{1}^T y\\ \text{subject to} & -y \preceq Ax - b \preceq y \end{array}$$

Penalty function approximation

minimize $\phi(r_1) + \cdots + \phi(r_m)$ subject to r = Ax - b

 $(A \in \mathbf{R}^{m \times n}, \phi : \mathbf{R} \to \mathbf{R} \text{ is a convex penalty function})$

examples



example (m = 100, n = 30): histogram of residuals for penalties

$$\phi(u) = |u|, \quad \phi(u) = u^2, \quad \phi(u) = \max\{0, |u| - a\}, \quad \phi(u) = -\log(1 - u^2)$$



shape of penalty function has large effect on distribution of residuals

Huber penalty function (with parameter M)

$$\phi_{\text{hub}}(u) = \begin{cases} u^2 & |u| \le M \\ M(2|u| - M) & |u| > M \end{cases}$$

linear growth for large u makes approximation less sensitive to outliers



- \blacksquare left: Huber penalty for M=1
- right: affine function $f(t) = \alpha + \beta t$ fitted to 42 points t_i , y_i (circles) using quadratic (dashed) and Huber (solid) penalty

 $\begin{array}{ll} \text{minimize} & \|x\|\\ \text{subject to} & Ax = b \end{array}$

 $(A \in \mathbf{R}^{m \times n} \text{ with } m \leq n, \|\cdot\| \text{ is a norm on } \mathbf{R}^n)$

interpretations of solution $x^* = \operatorname{argmin}_{Ax=b} \|x\|$:

- **geometric:** x^* is point in affine set $\{x \mid Ax = b\}$ with minimum distance to 0
- estimation: b = Ax are (perfect) measurements of x; x^* is smallest ('most plausible') estimate consistent with measurements
- **design:** x are design variables (inputs); b are required results (outputs)
 - x^{\star} is smallest ('most efficient') design that satisfies requirements

examples

• least-squares solution of linear equations $(\|\cdot\|_2)$:

can be solved via optimality conditions

$$2x + A^T \nu = 0, \qquad Ax = b$$

• minimum sum of absolute values $(\|\cdot\|_1)$: can be solved as an LP

minimize
$$\mathbf{1}^T y$$

subject to $-y \leq x \leq y$, $Ax = b$

tends to produce sparse solution x^\star

extension: least-penalty problem

minimize
$$\phi(x_1) + \dots + \phi(x_n)$$

subject to $Ax = b$

 $\phi: \mathbf{R} \rightarrow \mathbf{R}$ is convex penalty function

minimize (w.r.t. \mathbf{R}^2_+) (||Ax - b||, ||x||)

 $A \in \mathbf{R}^{m \times n}$, norms on \mathbf{R}^m and \mathbf{R}^n can be different

interpretation: find good approximation $Ax\approx b$ with small x

- estimation: linear measurement model y = Ax + v, with prior knowledge that ||x|| is small
- optimal design: small x is cheaper or more efficient, or the linear model y = Ax is only valid for small x
- robust approximation: good approximation $Ax \approx b$ with small x is less sensitive to errors in A than good approximation with large x

minimize $||Ax - b|| + \gamma ||x||$

 $\hfill \ensuremath{\,\,{\rm solution}}$ for $\gamma>0$ traces out optimal trade-off curve

• other common method: minimize $||Ax - b||^2 + \delta ||x||^2$ with $\delta > 0$

Tikhonov regularization

minimize
$$||Ax - b||_2^2 + \delta ||x||_2^2$$

can be solved as a least-squares problem

minimize
$$\left\| \begin{bmatrix} A \\ \sqrt{\delta}I \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_{2}^{2}$$

solution $x^{\star} = (A^T A + \delta I)^{-1} A^T b$

minimize (w.r.t. \mathbf{R}^{2}_{+}) $(\|\hat{x} - x_{cor}\|_{2}, \phi(\hat{x}))$

- $x \in \mathbf{R}^n$ is unknown signal
- $x_{cor} = x + v$ is (known) corrupted version of x, with additive noise v
- variable \hat{x} (reconstructed signal) is estimate of x
- $\phi : \mathbf{R}^n \to \mathbf{R}$ is regularization function or smoothing objective

examples: quadratic smoothing, total variation smoothing:

$$\phi_{\text{quad}}(\hat{x}) = \sum_{i=1}^{n-1} (\hat{x}_{i+1} - \hat{x}_i)^2, \qquad \phi_{\text{tv}}(\hat{x}) = \sum_{i=1}^{n-1} |\hat{x}_{i+1} - \hat{x}_i|$$

quadratic smoothing example



original signal x and noisy signal $x_{\rm cor}$



three solutions on trade-off curve $\|\hat{x} - x_{cor}\|_2$ versus $\phi_{quad}(\hat{x})$

total variation reconstruction example



quadratic smoothing smooths out noise and sharp transitions in signal



total variation smoothing preserves sharp transitions in signal

Geometrical Problems

- extremal volume ellipsoids
- centering
- placement and facility location.

Minimum volume ellipsoid around a set

Löwner-John ellipsoid of a set C: minimum volume ellipsoid \mathcal{E} s.t. $C \subseteq \mathcal{E}$

- parametrize \mathcal{E} as $\mathcal{E} = \{v \mid ||Av + b||_2 \le 1\}$; w.l.o.g. assume $A \in \mathbf{S}_{++}^n$
- $\operatorname{vol} \mathcal{E}$ is proportional to $\det A^{-1}$; to compute minimum volume ellipsoid,

minimize (over A, b)
$$\log \det A^{-1}$$

subject to $\sup_{v \in C} ||Av + b||_2 \le 1$

convex, but evaluating the constraint can be hard (for general C)

finite set
$$C = \{x_1, ..., x_m\}$$
:

minimize (over A, b) $\log \det A^{-1}$ subject to $\|Ax_i + b\|_2 \le 1, \quad i = 1, \dots, m$

also gives Löwner-John ellipsoid for polyhedron $Co\{x_1, \ldots, x_m\}$

Maximum volume inscribed ellipsoid

maximum volume ellipsoid ${\mathcal E}$ inside a convex set $C\subseteq {\mathbf R}^n$

- parametrize \mathcal{E} as $\mathcal{E} = \{Bu + d \mid ||u||_2 \leq 1\}$; w.l.o.g. assume $B \in \mathbf{S}_{++}^n$
- $\operatorname{vol} \mathcal{E}$ is proportional to $\det B$; can compute \mathcal{E} by solving

maximize
$$\log \det B$$

subject to $\sup_{\|u\|_2 \le 1} I_C(Bu+d) \le 0$

(where
$$I_C(x) = 0$$
 for $x \in C$ and $I_C(x) = \infty$ for $x \notin C$)

convex, but evaluating the constraint can be hard (for general C)

polyhedron $\{x \mid a_i^T x \le b_i, i = 1, ..., m\}$:

maximize
$$\log \det B$$

subject to $||Ba_i||_2 + a_i^T d \le b_i, \quad i = 1, \dots, m$

(constraint follows from $\sup_{\|u\|_2 \leq 1} a_i^T (Bu + d) = \|Ba_i\|_2 + a_i^T d$)

Efficiency of ellipsoidal approximations

 $C \subseteq \mathbf{R}^n$ convex, bounded, with nonempty interior

- Löwner-John ellipsoid, shrunk by a factor n, lies inside C
- **•** maximum volume inscribed ellipsoid, expanded by a factor n, covers C

example (for two polyhedra in \mathbf{R}^2)



factor n can be improved to \sqrt{n} if C is symmetric

Centering

some possible definitions of 'center' of a convex set C:

- center of largest inscribed ball ('Chebyshev center')
 - for polyhedron, can be computed via linear programming (page ??)
- center of maximum volume inscribed ellipsoid (page 19)



MVE center is invariant under affine coordinate transformations

Analytic center of a set inequalities

the analytic center of set of convex inequalities and linear equations

$$f_i(x) \le 0, \quad i = 1, \dots, m, \qquad Fx = g$$

is defined as the optimal point of

minimize
$$-\sum_{i=1}^{m} \log(-f_i(x))$$

subject to $Fx = g$

- more easily computed than MVE or Chebyshev center (see later)
- not just a property of the feasible set: two sets of inequalities can describe the same set, but have different analytic centers

analytic center of linear inequalities $a_i^T x \leq b_i$, $i = 1, \ldots, m$

 $x_{\rm ac}$ is minimizer of

$$\phi(x) = -\sum_{i=1}^{m} \log(b_i - a_i^T x)$$



inner and outer ellipsoids from analytic center:

$$\mathcal{E}_{\text{inner}} \subseteq \{x \mid a_i^T x \leq b_i, i = 1, \dots, m\} \subseteq \mathcal{E}_{\text{outer}}$$

where

$$\mathcal{E}_{\text{inner}} = \{ x \mid (x - x_{\text{ac}})^T \nabla^2 \phi(x_{\text{ac}}) (x - x_{\text{ac}} \le 1 \}$$

$$\mathcal{E}_{\text{outer}} = \{ x \mid (x - x_{\text{ac}})^T \nabla^2 \phi(x_{\text{ac}}) (x - x_{\text{ac}}) \le m(m-1) \}$$

Placement and facility location

- N points with coordinates $x_i \in \mathbf{R}^2$ (or \mathbf{R}^3)
- some positions x_i are given; the other x_i 's are variables
- for each pair of points, a cost function $f_{ij}(x_i, x_j)$

placement problem

minimize
$$\sum_{i \neq j} f_{ij}(x_i, x_j)$$

variables are positions of free points

interpretations

- points represent plants or warehouses; f_{ij} is transportation cost between facilities i and j
- points represent cells on an IC; f_{ij} represents wirelength

example: minimize $\sum_{(i,j)\in\mathcal{A}} h(||x_i - x_j||_2)$, with 6 free points, 27 links

optimal placement for h(z) = z, $h(z) = z^2$, $h(z) = z^4$



histograms of connection lengths $||x_i - x_j||_2$



Distance matrices

The problem of reconstructing an N-point Euclidean metric, given partial information on pairwise distances between points v_i, i = 1, ..., N can also be cast as an SDP, known as and Euclidean Distance Matrix Completion problem.

find
$$D$$

subject to $\mathbf{1}v^T + v\mathbf{1}^T - D \succeq 0$
 $D_{ij} = ||v_i - v_j||_2^2, \quad (i, j) \in S$
 $v \ge 0$

in the variables $D \in \mathbf{S}_n$ and $v \in \mathbf{R}^n$, on a subset $S \subset [1, N]^2$.

- We can add further constraints to this problem given additional structural info on the configuration.
- Applications in sensor networks, molecular conformation reconstruction etc...

Distance matrices . . .



[Dattorro, 2005] 3D map of the USA reconstructed from pairwise distances on 5000 points. Distances reconstructed from Latitude/Longitude data.

Distance matrices . . .



3D Caffeine. Reconstruct molecules from MRI data...

Mixing rates for Markov chains & maximum variance unfolding

- Let G = (V, E) be an **undirected graph** with n vertices and m edges.
- We define a **Markov chain** on this graph, and let $w_{ij} \ge 0$ be the transition rate for edge $(i, j) \in V$.



Let $\pi(t)$ be the state distribution at time t, its evolution is governed by the heat equation

$$d\pi(t) = -L\pi(t)dt$$

with

$$L_{ij} = \begin{cases} -w_{ij} & \text{if } i \neq j, \ (i,j) \in V \\ 0 & \text{if } (i,j) \notin V \\ \sum_{(i,k) \in V} w_{ik} & \text{if } i = j \end{cases}$$

the graph Laplacian matrix, which means

$$\pi(t) = e^{-Lt}\pi(0).$$

[Sun, Boyd, Xiao, and Diaconis, 2006]

Maximizing the mixing rate of the Markov chain means solving

$$\begin{array}{ll} \mbox{maximize} & t \\ \mbox{subject to} & L(w) \succeq t(\mathbf{I} - (1/n)\mathbf{1}\mathbf{1}^T) \\ & \sum_{(i,j) \in V} d_{ij}^2 w_{ij} \leq 1 \\ & w \geq 0 \end{array}$$

in the variable $w \in \mathbf{R}^m$, with (normalization) parameters $d_{ij}^2 \ge 0$.

Since L(w) is an affine function of the variable $w \in \mathbf{R}^m$, this is a semidefinite program in $w \in \mathbf{R}^m$.

[Weinberger and Saul, 2006, Sun et al., 2006]

The **dual** means solving

maximize
$$\operatorname{Tr}(X(\mathbf{I} - (1/n)\mathbf{1}\mathbf{1}^T))$$

subject to $X_{ii} - 2X_{ij} + X_{jj} \leq d_{ij}^2$, $(i, j) \in V$
 $X \succeq 0$,

in the variable $X \in \mathbf{S}_n$.

This is a maximum variance unfolding problem.





From [Sun et al., 2006]: we are given pairwise 3D distances for k-nearest neighbors in the point set on the right. We plot the maximum variance point set satisfying these pairwise distance bounds on the right.

References

- J. Dattorro. Convex optimization & Euclidean distance geometry. Meboo Publishing USA, 2005.
- J. Sun, S. Boyd, L. Xiao, and P. Diaconis. The fastest mixing Markov process on a graph and a connection to a maximum variance unfolding problem. *SIAM Review*, 48(4):681–699, 2006.
- K.Q. Weinberger and L.K. Saul. Unsupervised Learning of Image Manifolds by Semidefinite Programming. *International Journal of Computer Vision*, 70(1):77–90, 2006.