Optimization for the information and data sciences

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Geometric problems

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Geometric problems

- extremal volume ellipsoids
- centering
- classification
- 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 $\mathcal{E} = \{v \mid \|Av + b\|_2 \leq 1\}$; w.l.o.g. assume $A \in \mathcal{S}^n_{++}$
- **vol**$\mathcal{E}$ is proportional to $\det A^{-1}$; to compute minimum volume ellipsoid,

$$\begin{array}{ll} \text{minimize (over } A, b) & \log\det A^{-1} \\ \text{subject to} & \sup_{v \in C} \|Av + b\|_2 \leq 1 \end{array}$$

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

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

$$\begin{array}{ll} \text{minimize (over } A, b) & \log\det A^{-1} \\ \text{subject to} & \|Ax_i + b\|_2 \leq 1, \quad i = 1, \ldots, m \end{array}$$

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

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 $B \in \mathbf{S}^n_{++}$
- **vol**$\mathcal{E}$ is proportional to $\det B$; can compute $\mathcal{E}$ by solving

$$\begin{array}{ll} \text{maximize} & \log\det B \\ \text{subject to} & \sup_{\|u\|_2 \leq 1} I_C(Bu + d) \leq 0 \end{array}$$

(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 $\{x \mid a_i^T x \leq b_i,\ i = 1, \ldots, m\}$:

$$\begin{array}{ll} \text{maximize} & \log\det B \\ \text{subject to} & \|Ba_i\|_2 + a_i^T d \leq b_i, \quad i = 1, \ldots, m \end{array}$$

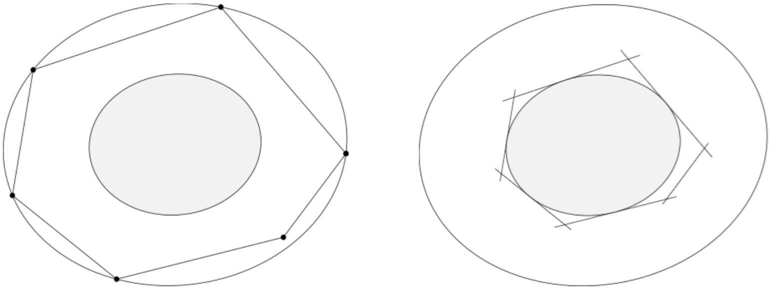
(constraint follows from $\sup_{\|u\|_2 \leq 1} a_i^T (Bu + d) = \|Ba_i\|_2 + a_i^T d$)

Efficiency of ellipsoidal approximations

$C \subseteq \mathbb{R}^n$ 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 $\mathbb{R}^2$)

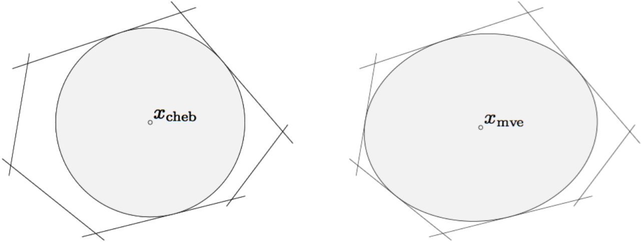


factor n can be improved to $\sqrt{n}$ if C is symmetric

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
- center of maximum volume inscribed ellipsoid



MVE center is invariant under affine coordinate transformations

Analytic center of a set of inequalities

the analytic center of set of convex inequalities and linear equations

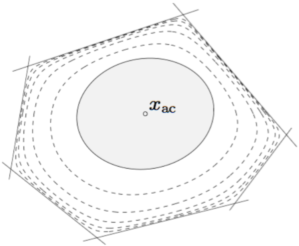
$$f_i(x) \leq 0, \quad i = 1, \ldots, m, \qquad Fx = g$$

is defined as the optimal point of

$$\begin{array}{ll} \text{minimize} & -\sum_{i=1}^m \log(-f_i(x)) \\ \text{subject to} & Fx = g \end{array}$$

- 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_{ac} is minimizer of

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

inner and outer ellipsoids from analytic center:

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

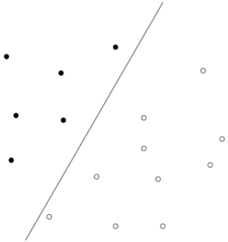
where

$$\begin{aligned}
\mathcal{E}_{\mathrm{inner}} &= \{x \mid (x - x_{\mathrm{ac}})^T \nabla^2 \phi(x_{\mathrm{ac}})(x - x_{\mathrm{ac}}) \leq 1\} \\
\mathcal{E}_{\mathrm{outer}} &= \{x \mid (x - x_{\mathrm{ac}})^T \nabla^2 \phi(x_{\mathrm{ac}})(x - x_{\mathrm{ac}}) \leq m(m-1)\}
\end{aligned}$$

Linear discrimination

separate two sets of points $\{x_1, \ldots, x_N\}$, $\{y_1, \ldots, y_M\}$ by a hyperplane:

$$a^T x_i + b > 0, \quad i = 1, \ldots, N, \qquad a^T y_i + b < 0, \quad i = 1, \ldots, M$$



homogeneous in a, b, hence equivalent to

$$a^T x_i + b \geq 1, \quad i = 1, \ldots, N, \qquad a^T y_i + b \leq -1, \quad i = 1, \ldots, M$$

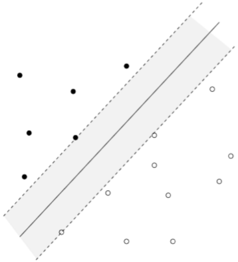
a set of linear inequalities in a, b

Robust linear discrimination

(Euclidean) distance between hyperplanes

$$\mathcal{H}_1 = \{z \mid a^T z + b = 1\}$$
$$\mathcal{H}_2 = \{z \mid a^T z + b = -1\}$$

is $\mathbf{dist}(\mathcal{H}_1, \mathcal{H}_2) = 2/\|a\|_2$



to separate two sets of points by maximum margin,

$$\begin{array}{ll} \text{minimize} & (1/2)\|a\|_2 \\ \text{subject to} & a^T x_i + b \geq 1, \quad i = 1, \ldots, N \\ & a^T y_i + b \leq -1, \quad i = 1, \ldots, M \end{array}$$

(after squaring objective) a QP in a, b

Lagrange dual of maximum margin separation problem

$$
\begin{array}{ll}
\text{maximize} & \mathbf{1}^T\lambda + \mathbf{1}^T\mu \\
\text{subject to} & 2\left\|\sum_{i=1}^N \lambda_i x_i - \sum_{i=1}^M \mu_i y_i\right\|_2 \leq 1 \\
& \mathbf{1}^T\lambda = \mathbf{1}^T\mu, \quad \lambda \succeq 0, \quad \mu \succeq 0
\end{array}
$$

from duality, optimal value is inverse of maximum margin of separation

interpretation

- change variables to $\theta_i = \lambda_i/\mathbf{1}^T\lambda$, $\gamma_i = \mu_i/\mathbf{1}^T\mu$, $t = 1/(\mathbf{1}^T\lambda + \mathbf{1}^T\mu)$
- invert objective to minimize $1/(\mathbf{1}^T\lambda + \mathbf{1}^T\mu) = t$

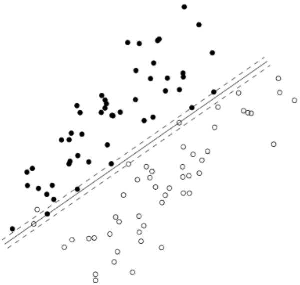
$$
\begin{array}{ll}
\text{minimize} & t \\
\text{subject to} & \left\|\sum_{i=1}^N \theta_i x_i - \sum_{i=1}^M \gamma_i y_i\right\|_2 \leq t \\
& \theta \succeq 0, \quad \mathbf{1}^T\theta = 1, \quad \gamma \succeq 0, \quad \mathbf{1}^T\gamma = 1
\end{array}
$$

optimal value is distance between convex hulls

Approximate linear separation of non-separable sets

$$\begin{array}{ll} \text{minimize} & \mathbf{1}^T u + \mathbf{1}^T v \\ \text{subject to} & a^T x_i + b \geq 1 - u_i, \quad i = 1, \ldots, N \\ & a^T y_i + b \leq -1 + v_i, \quad i = 1, \ldots, M \\ & u \succeq 0, \quad v \succeq 0 \end{array}$$

- an LP in a, b, u, v
- at optimum, $u_i = \max\{0, 1 - a^T x_i - b\}$, $v_i = \max\{0, 1 + a^T y_i + b\}$
- can be interpreted as a heuristic for minimizing #misclassified points

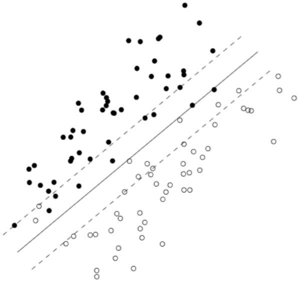


Support vector classifier

$$\begin{array}{ll} \text{minimize} & \|a\|_2 + \gamma(\mathbf{1}^T u + \mathbf{1}^T v) \\ \text{subject to} & a^T x_i + b \geq 1 - u_i, \quad i = 1, \ldots, N \\ & a^T y_i + b \leq -1 + v_i, \quad i = 1, \ldots, M \\ & u \succeq 0, \quad v \succeq 0 \end{array}$$

produces point on trade-off curve between inverse of margin $2/\|a\|_2$ and classification error, measured by total slack $\mathbf{1}^T u + \mathbf{1}^T v$

same example as previous page, with $\gamma = 0.1$:



Nonlinear discrimination

separate two sets of points by a nonlinear function:

$$f(x_i) > 0, \quad i = 1, \ldots, N, \qquad f(y_i) < 0, \quad i = 1, \ldots, M$$

- choose a linearly parametrized family of functions

$$f(z) = \theta^T F(z)$$

  $F = (F_1, \ldots, F_k) : \mathbb{R}^n \to \mathbb{R}^k$ are basis functions

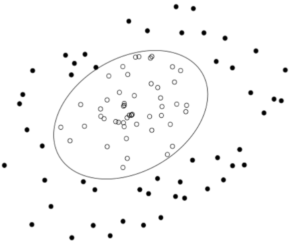
- solve a set of linear inequalities in θ:

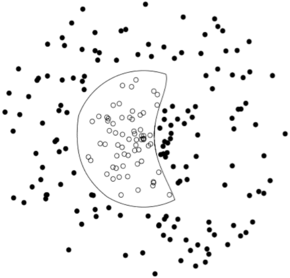
$$\theta^T F(x_i) \geq 1, \quad i = 1, \ldots, N, \qquad \theta^T F(y_i) \leq -1, \quad i = 1, \ldots, M$$

quadratic discrimination: $f(z) = z^T P z + q^T z + r$

$$x_i^T P x_i + q^T x_i + r \geq 1, \qquad y_i^T P y_i + q^T y_i + r \leq -1$$

can add additional constraints (e.g., $P \preceq -I$ to separate by an ellipsoid)
polynomial discrimination: $F(z)$ are all monomials up to a given degree





separation by ellipsoid

separation by 4th degree polynomial

Placement and facility location

- N points with coordinates $x_i \in \mathbb{R}^2$ (or $\mathbb{R}^3$)
- 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

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

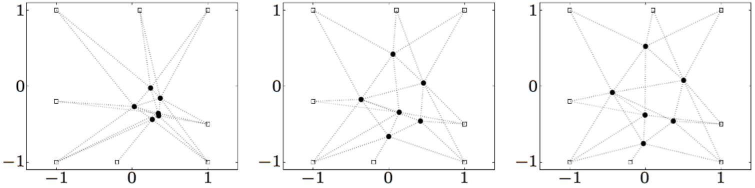
variables are positions of free points

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 $\|x_i - x_j\|_2$