

An introduction to convex methods for life science

Basics on convexity

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Outline

Convex set

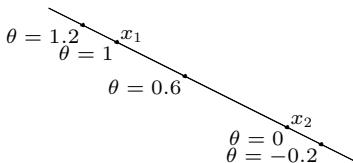
Convex functions

Convex problems

Affine set

line through x_1, x_2 : all points

$$x = \theta x_1 + (1 - \theta)x_2 \quad (\theta \in \mathbf{R})$$



affine set: contains the line through any two distinct points in the set

example: solution set of linear equations $\{x \mid Ax = b\}$

(conversely, every affine set can be expressed as solution set of system of linear equations)

Convex set

line segment between x_1 and x_2 : all points

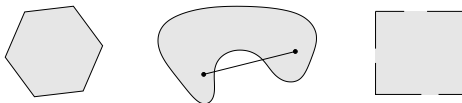
$$x = \theta x_1 + (1 - \theta)x_2$$

with $0 \leq \theta \leq 1$

convex set: contains line segment between any two points in the set

$$x_1, x_2 \in C, \quad 0 \leq \theta \leq 1 \quad \implies \quad \theta x_1 + (1 - \theta)x_2 \in C$$

examples (one convex, two nonconvex sets)



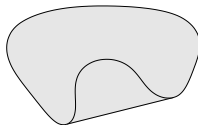
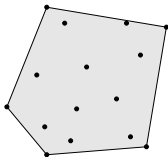
Convex combination and convex hull

convex combination of x_1, \dots, x_k : any point x of the form

$$x = \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_k x_k$$

with $\theta_1 + \dots + \theta_k = 1$, $\theta_i \geq 0$

convex hull $\text{conv } S$: set of all convex combinations of points in S

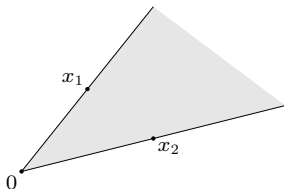


Convex cone

conic (nonnegative) combination of x_1 and x_2 : any point of the form

$$x = \theta_1 x_1 + \theta_2 x_2$$

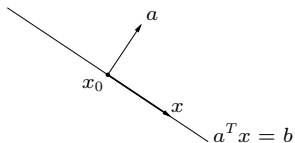
with $\theta_1 \geq 0$, $\theta_2 \geq 0$



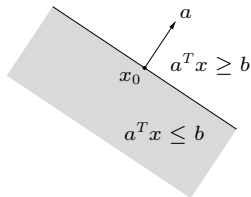
convex cone: set that contains all conic combinations of points in the set

Hyperplanes and halfspaces

hyperplane: set of the form $\{x \mid a^T x = b\}$ ($a \neq 0$)



halfspace: set of the form $\{x \mid a^T x \leq b\}$ ($a \neq 0$)



- a is the normal vector
- hyperplanes are affine and convex; halfspaces are convex

Euclidean balls and ellipsoids

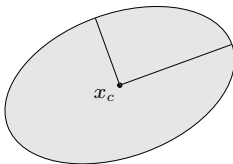
(Euclidean) ball with center x_c and radius r :

$$B(x_c, r) = \{x \mid \|x - x_c\|_2 \leq r\} = \{x_c + ru \mid \|u\|_2 \leq 1\}$$

ellipsoid: set of the form

$$\{x \mid (x - x_c)^T P^{-1} (x - x_c) \leq 1\}$$

with $P \in \mathbf{S}_{++}^n$ (i.e., P symmetric positive definite)



other representation: $\{x_c + Au \mid \|u\|_2 \leq 1\}$ with A square and nonsingular

Norm balls and norm cones

norm: a function $\|\cdot\|$ that satisfies

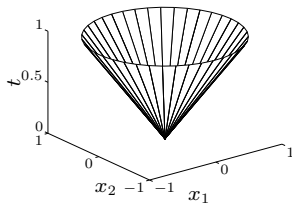
- $\|x\| \geq 0$; $\|x\| = 0$ if and only if $x = 0$
- $\|tx\| = |t| \|x\|$ for $t \in \mathbf{R}$
- $\|x + y\| \leq \|x\| + \|y\|$

notation: $\|\cdot\|$ is general (unspecified) norm; $\|\cdot\|_{\text{symb}}$ is particular norm

norm ball with center x_c and radius r : $\{x \mid \|x - x_c\| \leq r\}$

norm cone: $\{(x, t) \mid \|x\| \leq t\}$

Euclidean norm cone is called second-order cone



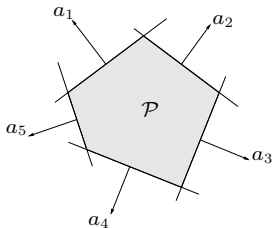
norm balls and cones are convex

Polyhedra

solution set of finitely many linear inequalities and equalities

$$Ax \preceq b, \quad Cx = d$$

($A \in \mathbf{R}^{m \times n}$, $C \in \mathbf{R}^{p \times n}$, \preceq is componentwise inequality)



polyhedron is intersection of finite number of halfspaces and hyperplanes

Positive semidefinite cone

notation:

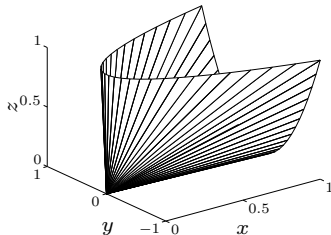
- \mathbf{S}^n is set of symmetric $n \times n$ matrices
- $\mathbf{S}_+^n = \{X \in \mathbf{S}^n \mid X \succeq 0\}$: positive semidefinite $n \times n$ matrices

$$X \in \mathbf{S}_+^n \iff z^T X z \geq 0 \text{ for all } z$$

\mathbf{S}_+^n is a convex cone

- $\mathbf{S}_{++}^n = \{X \in \mathbf{S}^n \mid X \succ 0\}$: positive definite $n \times n$ matrices

example: $\begin{bmatrix} x & y \\ y & z \end{bmatrix} \in \mathbf{S}_+^2$



Operations that preserve convexity

practical methods for establishing convexity of a set C

1. apply definition

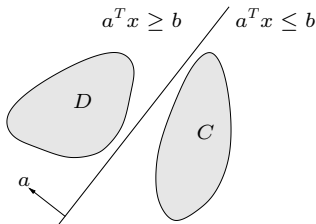
$$x_1, x_2 \in C, \quad 0 \leq \theta \leq 1 \quad \implies \quad \theta x_1 + (1 - \theta)x_2 \in C$$

2. show that C is obtained from simple convex sets (hyperplanes, halfspaces, norm balls, . . .) by operations that preserve convexity
 - intersection
 - affine functions
 - perspective function
 - linear-fractional functions

Separating hyperplane theorem

if C and D are disjoint convex sets, then there exists $a \neq 0$, b such that

$$a^T x \leq b \text{ for } x \in C, \quad a^T x \geq b \text{ for } x \in D$$



the hyperplane $\{x \mid a^T x = b\}$ separates C and D

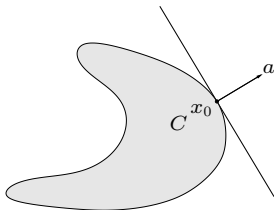
strict separation requires additional assumptions (*e.g.*, C is closed, D is a singleton)

Supporting hyperplane theorem

supporting hyperplane to set C at boundary point x_0 :

$$\{x \mid a^T x = a^T x_0\}$$

where $a \neq 0$ and $a^T x \leq a^T x_0$ for all $x \in C$



supporting hyperplane theorem: if C is convex, then there exists a supporting hyperplane at every boundary point of C

Outline

Convex set

Convex functions

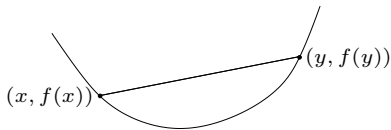
Convex problems

Definition

$f : \mathbf{R}^n \rightarrow \mathbf{R}$ is convex if $\mathbf{dom} f$ is a convex set and

$$f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y)$$

for all $x, y \in \mathbf{dom} f$, $0 \leq \theta \leq 1$



- f is concave if $-f$ is convex
- f is strictly convex if $\mathbf{dom} f$ is convex and

$$f(\theta x + (1 - \theta)y) < \theta f(x) + (1 - \theta)f(y)$$

for $x, y \in \mathbf{dom} f$, $x \neq y$, $0 < \theta < 1$

Examples on \mathbf{R}

convex:

- affine: $ax + b$ on \mathbf{R} , for any $a, b \in \mathbf{R}$
- exponential: e^{ax} , for any $a \in \mathbf{R}$
- powers: x^α on \mathbf{R}_{++} , for $\alpha \geq 1$ or $\alpha \leq 0$
- powers of absolute value: $|x|^p$ on \mathbf{R} , for $p \geq 1$
- negative entropy: $x \log x$ on \mathbf{R}_{++}

concave:

- affine: $ax + b$ on \mathbf{R} , for any $a, b \in \mathbf{R}$
- powers: x^α on \mathbf{R}_{++} , for $0 \leq \alpha \leq 1$
- logarithm: $\log x$ on \mathbf{R}_{++}

Examples on \mathbf{R}^n and $\mathbf{R}^{m \times n}$

affine functions are convex and concave; all norms are convex

examples on \mathbf{R}^n

- affine function $f(x) = a^T x + b$
- norms: $\|x\|_p = (\sum_{i=1}^n |x_i|^p)^{1/p}$ for $p \geq 1$; $\|x\|_\infty = \max_k |x_k|$

examples on $\mathbf{R}^{m \times n}$ ($m \times n$ matrices)

- affine function

$$f(X) = \text{tr}(A^T X) + b = \sum_{i=1}^m \sum_{j=1}^n A_{ij} X_{ij} + b$$

- spectral (maximum singular value) norm

$$f(X) = \|X\|_2 = \sigma_{\max}(X) = (\lambda_{\max}(X^T X))^{1/2}$$

Restriction of a convex function to a line

$f : \mathbf{R}^n \rightarrow \mathbf{R}$ is convex if and only if the function $g : \mathbf{R} \rightarrow \mathbf{R}$,

$$g(t) = f(x + tv), \quad \text{dom } g = \{t \mid x + tv \in \text{dom } f\}$$

is convex (in t) for any $x \in \text{dom } f$, $v \in \mathbf{R}^n$

can check convexity of f by checking convexity of functions of one variable

example. $f : \mathbf{S}^n \rightarrow \mathbf{R}$ with $f(X) = \log \det X$, $\text{dom } f = \mathbf{S}_{++}^n$

$$\begin{aligned} g(t) = \log \det(X + tV) &= \log \det X + \log \det(I + tX^{-1/2}VX^{-1/2}) \\ &= \log \det X + \sum_{i=1}^n \log(1 + t\lambda_i) \end{aligned}$$

where λ_i are the eigenvalues of $X^{-1/2}VX^{-1/2}$

g is concave in t (for any choice of $X \succ 0$, V); hence f is concave

Extended-value extension

extended-value extension \tilde{f} of f is

$$\tilde{f}(x) = f(x), \quad x \in \mathbf{dom} f, \quad \tilde{f}(x) = \infty, \quad x \notin \mathbf{dom} f$$

often simplifies notation; for example, the condition

$$0 \leq \theta \leq 1 \implies \tilde{f}(\theta x + (1 - \theta)y) \leq \theta \tilde{f}(x) + (1 - \theta) \tilde{f}(y)$$

(as an inequality in $\mathbf{R} \cup \{\infty\}$), means the same as the two conditions

- $\mathbf{dom} f$ is convex
- for $x, y \in \mathbf{dom} f$,

$$0 \leq \theta \leq 1 \implies f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y)$$

First-order condition

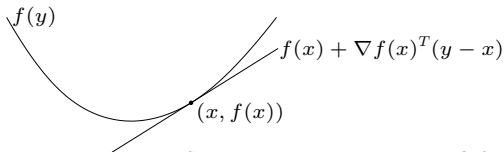
f is **differentiable** if $\text{dom } f$ is open and the gradient

$$\nabla f(x) = \left(\frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2}, \dots, \frac{\partial f(x)}{\partial x_n} \right)$$

exists at each $x \in \text{dom } f$

1st-order condition: differentiable f with convex domain is convex iff

$$f(y) \geq f(x) + \nabla f(x)^T(y - x) \quad \text{for all } x, y \in \text{dom } f$$



first-order approximation of f is global underestimator

Second-order conditions

f is **twice differentiable** if $\text{dom } f$ is open and the Hessian $\nabla^2 f(x) \in \mathbf{S}^n$,

$$\nabla^2 f(x)_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}, \quad i, j = 1, \dots, n,$$

exists at each $x \in \text{dom } f$

2nd-order conditions: for twice differentiable f with convex domain

- f is convex if and only if

$$\nabla^2 f(x) \succeq 0 \quad \text{for all } x \in \text{dom } f$$

- if $\nabla^2 f(x) \succ 0$ for all $x \in \text{dom } f$, then f is strictly convex

Examples

quadratic function: $f(x) = (1/2)x^T Px + q^T x + r$ (with $P \in \mathbf{S}^n$)

$$\nabla f(x) = Px + q, \quad \nabla^2 f(x) = P$$

convex if $P \succeq 0$

least-squares objective: $f(x) = \|Ax - b\|_2^2$

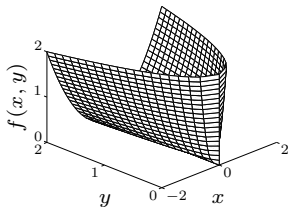
$$\nabla f(x) = 2A^T(Ax - b), \quad \nabla^2 f(x) = 2A^T A$$

convex (for any A)

quadratic-over-linear: $f(x, y) = x^2/y$

$$\nabla^2 f(x, y) = \frac{2}{y^3} \begin{bmatrix} y \\ -x \end{bmatrix} \begin{bmatrix} y \\ -x \end{bmatrix}^T \succeq 0$$

convex for $y > 0$



log-sum-exp: $f(x) = \log \sum_{k=1}^n \exp x_k$ is convex

$$\nabla^2 f(x) = \frac{1}{\mathbf{1}^T z} \mathbf{diag}(z) - \frac{1}{(\mathbf{1}^T z)^2} z z^T \quad (z_k = \exp x_k)$$

to show $\nabla^2 f(x) \succeq 0$, we must verify that $v^T \nabla^2 f(x) v \geq 0$ for all v :

$$v^T \nabla^2 f(x) v = \frac{(\sum_k z_k v_k^2)(\sum_k z_k) - (\sum_k v_k z_k)^2}{(\sum_k z_k)^2} \geq 0$$

since $(\sum_k v_k z_k)^2 \leq (\sum_k z_k v_k^2)(\sum_k z_k)$ (from Cauchy-Schwarz inequality)

geometric mean: $f(x) = (\prod_{k=1}^n x_k)^{1/n}$ on \mathbf{R}_{++}^n is concave

(similar proof as for log-sum-exp)

Epigraph and sublevel set

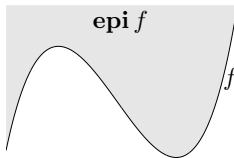
α -sublevel set of $f : \mathbf{R}^n \rightarrow \mathbf{R}$:

$$C_\alpha = \{x \in \text{dom } f \mid f(x) \leq \alpha\}$$

sublevel sets of convex functions are convex (converse is false)

epigraph of $f : \mathbf{R}^n \rightarrow \mathbf{R}$:

$$\text{epi } f = \{(x, t) \in \mathbf{R}^{n+1} \mid x \in \text{dom } f, f(x) \leq t\}$$



f is convex if and only if **epi** f is a convex set

Jensen's inequality

basic inequality: if f is convex, then for $0 \leq \theta \leq 1$,

$$f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y)$$

extension: if f is convex, then

$$f(\mathbf{E} z) \leq \mathbf{E} f(z)$$

for any random variable z

basic inequality is special case with discrete distribution

$$\mathbf{prob}(z = x) = \theta, \quad \mathbf{prob}(z = y) = 1 - \theta$$

Operations that preserve convexity

practical methods for establishing convexity of a function

1. verify definition (often simplified by restricting to a line)
2. for twice differentiable functions, show $\nabla^2 f(x) \succeq 0$
3. show that f is obtained from simple convex functions by operations that preserve convexity
 - nonnegative weighted sum
 - composition with affine function
 - pointwise maximum and supremum
 - composition
 - minimization
 - perspective

Positive weighted sum & composition with affine function

nonnegative multiple: αf is convex if f is convex, $\alpha \geq 0$

sum: $f_1 + f_2$ convex if f_1, f_2 convex (extends to infinite sums, integrals)

composition with affine function: $f(Ax + b)$ is convex if f is convex

examples

- log barrier for linear inequalities

$$f(x) = - \sum_{i=1}^m \log(b_i - a_i^T x), \quad \text{dom } f = \{x \mid a_i^T x < b_i, i = 1, \dots, m\}$$

- (any) norm of affine function: $f(x) = \|Ax + b\|$

Pointwise maximum

if f_1, \dots, f_m are convex, then $f(x) = \max\{f_1(x), \dots, f_m(x)\}$ is convex

examples

- piecewise-linear function: $f(x) = \max_{i=1, \dots, m}(a_i^T x + b_i)$ is convex
- sum of r largest components of $x \in \mathbf{R}^n$:

$$f(x) = x_{[1]} + x_{[2]} + \dots + x_{[r]}$$

is convex ($x_{[i]}$ is i th largest component of x)

proof:

$$f(x) = \max\{x_{i_1} + x_{i_2} + \dots + x_{i_r} \mid 1 \leq i_1 < i_2 < \dots < i_r \leq n\}$$

Pointwise supremum

if $f(x, y)$ is convex in x for each $y \in \mathcal{A}$, then

$$g(x) = \sup_{y \in \mathcal{A}} f(x, y)$$

is convex

examples

- support function of a set C : $S_C(x) = \sup_{y \in C} y^T x$ is convex
- distance to farthest point in a set C :

$$f(x) = \sup_{y \in C} \|x - y\|$$

- maximum eigenvalue of symmetric matrix: for $X \in \mathbf{S}^n$,

$$\lambda_{\max}(X) = \sup_{\|y\|_2=1} y^T X y$$

Composition with scalar functions

composition of $g : \mathbf{R}^n \rightarrow \mathbf{R}$ and $h : \mathbf{R} \rightarrow \mathbf{R}$:

$$f(x) = h(g(x))$$

f is convex if $\begin{array}{l} g \text{ convex, } h \text{ convex, } \tilde{h} \text{ nondecreasing} \\ g \text{ concave, } h \text{ convex, } \tilde{h} \text{ nonincreasing} \end{array}$

- proof (for $n = 1$, differentiable g, h)

$$f''(x) = h''(g(x))g'(x)^2 + h'(g(x))g''(x)$$

- note: monotonicity must hold for extended-value extension \tilde{h}

examples

- $\exp g(x)$ is convex if g is convex
- $1/g(x)$ is convex if g is concave and positive

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Convex problems

Optimization problem in standard form

$$\begin{array}{ll}\text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m \\ & h_i(x) = 0, \quad i = 1, \dots, p\end{array}$$

- $x \in \mathbf{R}^n$ is the optimization variable
- $f_0 : \mathbf{R}^n \rightarrow \mathbf{R}$ is the objective or cost function
- $f_i : \mathbf{R}^n \rightarrow \mathbf{R}$, $i = 1, \dots, m$, are the inequality constraint functions
- $h_i : \mathbf{R}^n \rightarrow \mathbf{R}$ are the equality constraint functions

optimal value:

$$p^* = \inf\{f_0(x) \mid f_i(x) \leq 0, \quad i = 1, \dots, m, \quad h_i(x) = 0, \quad i = 1, \dots, p\}$$

- $p^* = \infty$ if problem is infeasible (no x satisfies the constraints)
- $p^* = -\infty$ if problem is unbounded below

Implicit constraints

the standard form optimization problem has an **implicit constraint**

$$x \in \mathcal{D} = \bigcap_{i=0}^m \text{dom } f_i \cap \bigcap_{i=1}^p \text{dom } h_i,$$

- we call \mathcal{D} the **domain** of the problem
- the constraints $f_i(x) \leq 0$, $h_i(x) = 0$ are the explicit constraints
- a problem is **unconstrained** if it has no explicit constraints ($m = p = 0$)

example:

$$\text{minimize } f_0(x) = -\sum_{i=1}^k \log(b_i - a_i^T x)$$

is an unconstrained problem with implicit constraints $a_i^T x < b_i$

Feasibility problem

$$\begin{array}{ll}\text{find} & x \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m \\ & h_i(x) = 0, \quad i = 1, \dots, p\end{array}$$

can be considered a special case of the general problem with $f_0(x) = 0$:

$$\begin{array}{ll}\text{minimize} & 0 \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m \\ & h_i(x) = 0, \quad i = 1, \dots, p\end{array}$$

- $p^* = 0$ if constraints are feasible; any feasible x is optimal
- $p^* = \infty$ if constraints are infeasible

Convex optimization problem

standard form convex optimization problem

$$\begin{array}{ll}\text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m \\ & a_i^T x = b_i, \quad i = 1, \dots, p\end{array}$$

- f_0, f_1, \dots, f_m are convex; equality constraints are affine
- problem is *quasiconvex* if f_0 is quasiconvex (and f_1, \dots, f_m convex)

often written as

$$\begin{array}{ll}\text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m \\ & Ax = b\end{array}$$

important property: feasible set of a convex optimization problem is convex

example

$$\begin{array}{ll}\text{minimize} & f_0(x) = x_1^2 + x_2^2 \\ \text{subject to} & f_1(x) = x_1/(1 + x_2^2) \leq 0 \\ & h_1(x) = (x_1 + x_2)^2 = 0\end{array}$$

- f_0 is convex; feasible set $\{(x_1, x_2) \mid x_1 = -x_2 \leq 0\}$ is convex
- not a convex problem (according to our definition): f_1 is not convex, h_1 is not affine
- equivalent (but not identical) to the convex problem

$$\begin{array}{ll}\text{minimize} & x_1^2 + x_2^2 \\ \text{subject to} & x_1 \leq 0 \\ & x_1 + x_2 = 0\end{array}$$

Local and global optima

any locally optimal point of a convex problem is (globally) optimal

proof: suppose x is locally optimal and y is optimal with $f_0(y) < f_0(x)$

x locally optimal means there is an $R > 0$ such that

$$z \text{ feasible, } \|z - x\|_2 \leq R \implies f_0(z) \geq f_0(x)$$

consider $z = \theta y + (1 - \theta)x$ with $\theta = R/(2\|y - x\|_2)$

- $\|y - x\|_2 > R$, so $0 < \theta < 1/2$
- z is a convex combination of two feasible points, hence also feasible
- $\|z - x\|_2 = R/2$ and

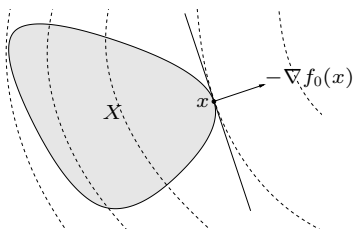
$$f_0(z) \leq \theta f_0(y) + (1 - \theta)f_0(x) < f_0(x)$$

which contradicts our assumption that x is locally optimal

Optimality criterion for differentiable f_0

x is optimal if and only if it is feasible and

$$\nabla f_0(x)^T(y - x) \geq 0 \quad \text{for all feasible } y$$



if nonzero, $\nabla f_0(x)$ defines a supporting hyperplane to feasible set X at x

- **unconstrained problem:** x is optimal if and only if

$$x \in \text{dom } f_0, \quad \nabla f_0(x) = 0$$

- **equality constrained problem**

$$\text{minimize } f_0(x) \quad \text{subject to } Ax = b$$

x is optimal if and only if there exists a ν such that

$$x \in \text{dom } f_0, \quad Ax = b, \quad \nabla f_0(x) + A^T \nu = 0$$

- **minimization over nonnegative orthant**

$$\text{minimize } f_0(x) \quad \text{subject to } x \succeq 0$$

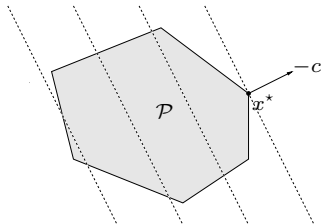
x is optimal if and only if

$$x \in \text{dom } f_0, \quad x \succeq 0, \quad \begin{cases} \nabla f_0(x)_i \geq 0 & x_i = 0 \\ \nabla f_0(x)_i = 0 & x_i > 0 \end{cases}$$

Linear program (LP)

$$\begin{array}{ll}\text{minimize} & c^T x + d \\ \text{subject to} & Gx \preceq h \\ & Ax = b\end{array}$$

- convex problem with affine objective and constraint functions
- feasible set is a polyhedron



Examples

diet problem: choose quantities x_1, \dots, x_n of n foods

- one unit of food j costs c_j , contains amount a_{ij} of nutrient i
- healthy diet requires nutrient i in quantity at least b_i

to find cheapest healthy diet,

$$\begin{array}{ll}\text{minimize} & c^T x \\ \text{subject to} & Ax \succeq b, \quad x \succeq 0\end{array}$$

piecewise-linear minimization

$$\text{minimize} \quad \max_{i=1, \dots, m} (a_i^T x + b_i)$$

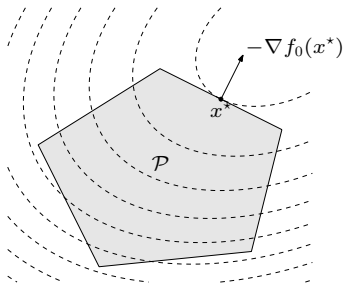
equivalent to an LP

$$\begin{array}{ll}\text{minimize} & t \\ \text{subject to} & a_i^T x + b_i \leq t, \quad i = 1, \dots, m\end{array}$$

Quadratic program (QP)

$$\begin{array}{ll}\text{minimize} & (1/2)x^T Px + q^T x + r \\ \text{subject to} & Gx \preceq h \\ & Ax = b\end{array}$$

- $P \in \mathbf{S}_{+}^n$, so objective is convex quadratic
- minimize a convex quadratic function over a polyhedron



Examples

least-squares

$$\text{minimize} \quad \|Ax - b\|_2^2$$

- analytical solution $x^* = A^\dagger b$ (A^\dagger is pseudo-inverse)
- can add linear constraints, *e.g.*, $l \preceq x \preceq u$

linear program with random cost

$$\begin{array}{ll} \text{minimize} & \bar{c}^T x + \gamma x^T \Sigma x = \mathbf{E} c^T x + \gamma \mathbf{var}(c^T x) \\ \text{subject to} & Gx \preceq h, \quad Ax = b \end{array}$$

- c is random vector with mean \bar{c} and covariance Σ
- hence, $c^T x$ is random variable with mean $\bar{c}^T x$ and variance $x^T \Sigma x$
- $\gamma > 0$ is risk aversion parameter; controls the trade-off between expected cost and variance (risk)