Introduction to Optimization

Romain Couillet and Ronald Phlypo

December 3, 2020

Outline

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Main objective

Objective of the class: solve the problem

$$\text{Find } x^\star \in \operatorname{argmin}_{x \in \Omega \subset \mathcal{X}} f(x) \tag{1}$$

for some function $f : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$.

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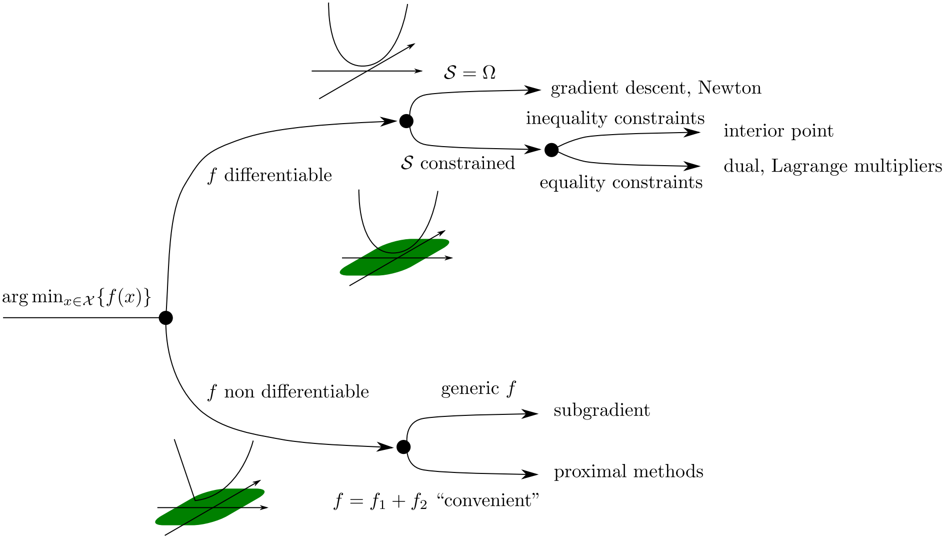
- f is the *cost*, *penalty*, or *objective* function;
- $\Omega = \mathcal{S} \cap \mathcal{X}$ is the set of constraints $\mathcal{S}$ restricted to $\mathcal{X}$.

Specifying f



Examples: the Lab Sessions

Example (1. Portfolio Optimization)

Setting:

- n assets;
- at time t, return $[x_t]_i$ for asset i, with $\mathbb{E}[x_t] = \mu$ and $\mathrm{Cov}[x_t] = C$;
- investment of wealth 1 across assets $[w]_1, \ldots, [w]_n$, $\sum_{i=1}^n [w]_i = 1$.

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- Optimal expected gain:

$$\operatorname{argmax}_{w \in \mathbb{R}^n} \mathbb{E}[w^\mathsf{T} x_t] = w^\mathsf{T} \mu, \text{ such that } \sum_{i=1}^n [w]_i = 1.$$

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- Risk minimization:

$$\mathrm{argmin}_{w \in \mathbb{R}^n} \mathbb{E}[|w^\mathsf{T}(x_t - \mu)|^2], \text{ such that } \sum_{i=1}^n [w]_i = 1.$$

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$$\operatorname{argmin}_{w \in \mathbb{R}^n} \mathbb{E}[|w^\mathsf{T}(x_t - \mu)|^2], \text{ such that } \sum_{i=1}^n [w]_i = 1.$$

- Risk minimization under constrained expected gain g:

$$\operatorname{argmin}_{w \in \mathbb{R}^n} \mathbb{E}[|w^\mathsf{T}(x_t - \mu)|^2], \text{ such that } \sum_{i=1}^n [w]_i = 1 \text{ and } \mathbb{E}[w^\mathsf{T} x_t] \geq g.$$

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- Risk minimization with non-negativity constraint:

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Overview:

- Without inequality constraint, Lagrange multipliers give the solution:

$$w^\star = \frac{C^{-1}1_n}{1_n^\top C^{-1}1_n}.$$

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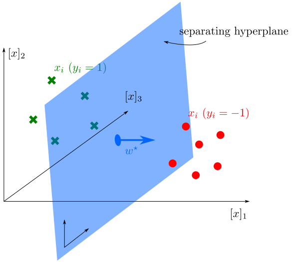
- With inequality constraint, interior point method (Lab Session 1), or proximal point method (Lab Session 2).

Example (2. Support Vector Machines)

Setting:

- Data points and labels $(x_1, y_1), \ldots, (x_m, y_m) \in \mathbb{R}^n \times \{\pm 1\}$;
- Separating hyperplane of $\mathbb{R}^n$ of the form $\mathcal{H} = \{x \mid x^\mathsf{T} w^\star + b^\star = 0\}$.



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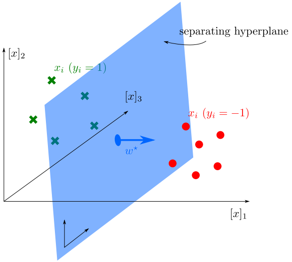

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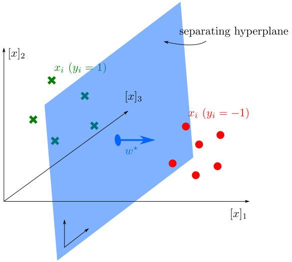

Objective: Maximize hyperplane "margin", or equivalently

$$(w^\star, b^\star) \in \operatorname{argmin}_{w,b \in \mathbb{R}^n} \left\{ \|w\|^2 \right\} \text{ such that } y_i(w^\mathsf{T} x_i + b) \geq 1.$$

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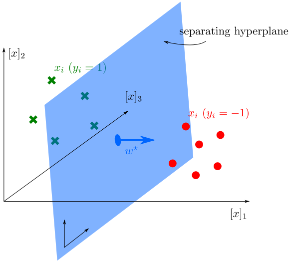

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Why? Distance between "supporting" hyperplanes $\mathcal{H}_{\pm 1} : x^\mathsf{T} w^\star + b^\star = \pm 1$ for all $\|x_{+1} - x_{-1}\|$, $x_{\pm 1} \in \mathcal{H}_{\pm 1}$: implies $(x_{+1} - x_{-1})^\mathsf{T} w^\star = 2$. Distance max for $\|w^\star\|$ min.

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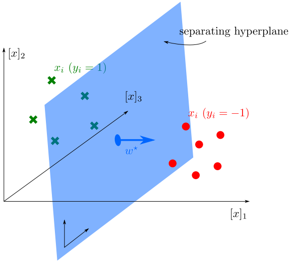

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But argmin can be empty! Relaxation to "soft-margin" SVM:

$$(w^\star, b^\star) \in \operatorname{argmin}_{w,b \in \mathbb{R}^p} \left\{ \frac{1}{m} \sum_{i=1}^{m} \max(0, 1 - y_i[w^\mathsf{T} x_i + b]) + \lambda \|w\|^2 \right\}$$

for some $\lambda > 0$.

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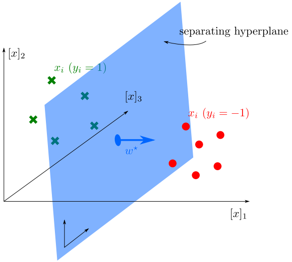

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Solution: Interior point or proximal methods.

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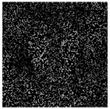


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- retrieve $x \in \mathbb{R}^n$ from $y = Ax \in \mathbb{R}^p$, $p \ll n$, with x a *sparse* vector;

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 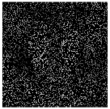 

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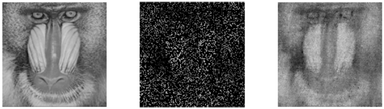

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 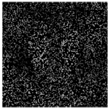 

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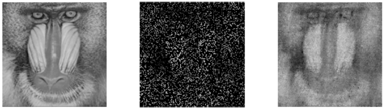

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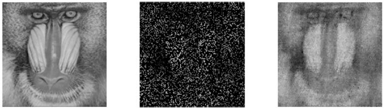

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Solution: Proximal methods and the *Douglas-Rachford splitting* algorithm.

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Convex Sets

Definition (Convex Set)

$\mathcal{C} \subset \mathcal{X}$ convex iif $\forall x, y \in \mathcal{C}$ and $\forall \lambda \in [0, 1]$,

$$(1-\lambda)x + \lambda y = x + \lambda(y - x) \in \mathcal{C}.$$

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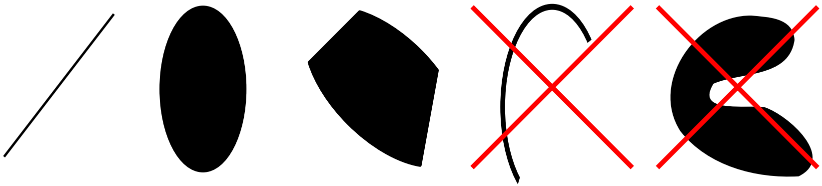

Figure: Convex sets and non-convex sets (stroke out).

Convex Sets: basic properties

Remark (Ensemble manipulations on convex sets)

For convex sets $\mathcal{C}_1$, $\mathcal{C}_2$,

- $\mathcal{C}_i$ *can be open, closed, bounded, unbounded.*
- $\mathcal{C}_1 \cap \mathcal{C}_2$ *is convex.*
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Remark (List of convex sets)

The following ensembles are convex:

- *line, segment, half-line,* $\mathbb{R}^n$
- *a vector subspace*
- *hyperplanes* $\{x,\ x^\mathsf{T} a = b\}$, *half-spaces* $\{x,\ x^\mathsf{T} a \leq b\}$
- *balls* $\mathcal{B}(x_c; r) \equiv \{x,\ \|x - x_c\| \leq r\}$ *and ellipsoids* $\{x,\ (x - x_c)^\mathsf{T} P^{-1}(x - x_c) \leq r\}$.

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Exercise (1. Ball convexity)

Show that $\mathcal{B}(x_c; r) \equiv \{x,\ \|x - x_c\| \leq r\}$ *is convex.*

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Proof of ball convexity.

Let $x, y \in \mathcal{B}(x_c; r)$. Then,

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$\square$

Exercise (2. Polyhedron convexity)

For $A \in \mathbb{R}^{l\times n}$, $B \in \mathbb{R}^{m\times n}$ *and* $b \in \mathbb{R}^l$, $d \in \mathbb{R}^m$, *show the convexity of polyhedron*

$$\mathcal{P} = \{x,\ Ax \leq b,\ Cx = d\}\,.$$

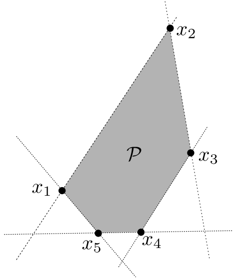

Figure: A polyhedron.

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The set of convex combinations of $x_1, \ldots, x_k \in \mathcal{S}$ is the set

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Property (Convex sets and convex hulls)

$\operatorname{conv}(\mathcal{X})$ *is the smallest convex set containing* $\mathcal{X}$*:* $\mathcal{X}$ *is convex iif* $\mathcal{X} = \operatorname{conv}(\mathcal{X})$.

Outline

Convex Function

Definition (Epigraph of a function)

The epigraph of $f : \mathcal{X} \to \mathbb{R}$ is the set

$$\mathrm{epi}(f) = \{(x, c) \in \mathcal{X} \times \mathbb{R},\ f(x) \leq c\}\,.$$

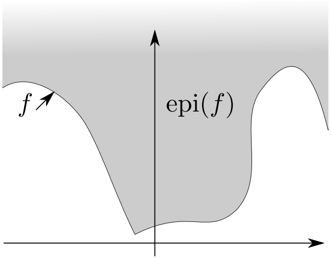

Figure: Epigraph of a function $f : \mathbb{R} \to \mathbb{R}$.

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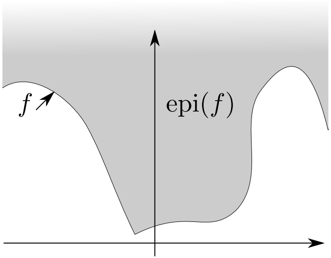

Figure: Epigraph of a function $f : \mathbb{R} \to \mathbb{R}$.

Definition (Convex function)

A function $f : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ is convex iif $\mathrm{epi}(f)$ is a convex set.

Convex Function

Property (Convex function)

$f : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ is convex iif, for all $x, y \in \mathcal{X}$ and $\lambda \in [0, 1]$,

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda)f(y).$$

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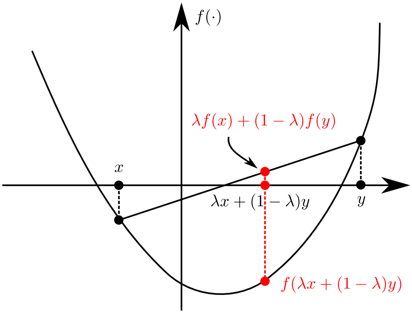

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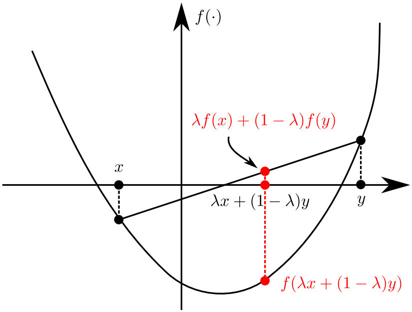

Proof.

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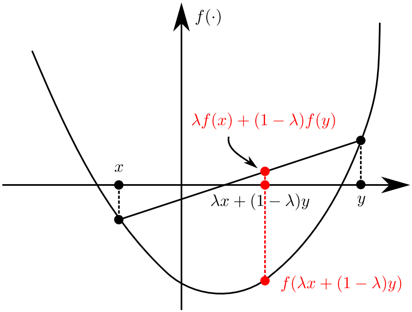

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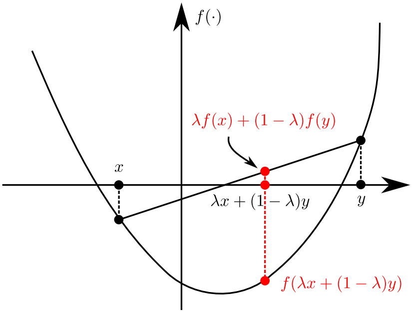

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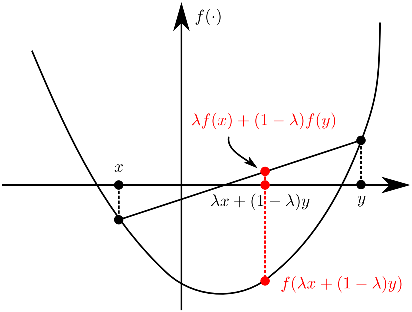

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$\Leftarrow$ For $x, y \in \mathcal{X}$, $(\lambda x + (1-\lambda)y, \lambda f(x) + (1-\lambda)f(y)) \in \mathrm{epi}(f)$ and so $\mathrm{epi}(f)$ is convex.

Differentiable convex function

Reminder. For f *differentiable at* x, $\nabla f(x) = \left\{ \frac{\partial f}{\partial x_i}(x) \right\}_{i=1}^{n}$.

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The domain of $f : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ is the set $\mathrm{dom}(f) = \{x, f(x) < +\infty\}$.

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Theorem (First order conditions)

For $f : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ *differentiable in its domain,* f *convex iif,* $\forall x, y \in \mathrm{dom}(f)$*,*

$$f(y) \geq f(x) + \nabla f(x)^{\mathsf{T}}(y - x).$$

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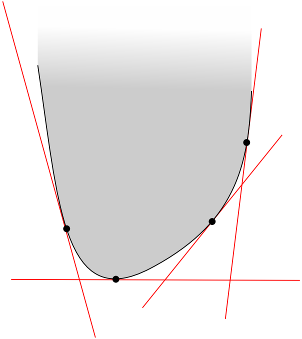
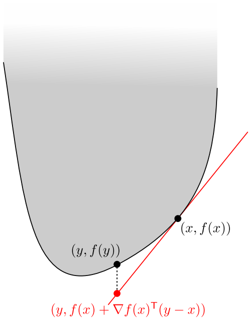
Differentiable f: f convex iif all tangent hyperplanes of $\mathrm{epi}(f)$ are below the epigraph.





Differentiable convex function

Proof.

$\Rightarrow$ f convex implies, for $\lambda \in [0,1]$, $x, y \in \mathcal{X}$,

$$f(\lambda x + (1-\lambda)y) = f(y + \lambda(x-y)) \leq \lambda f(x) + (1-\lambda)f(y) = \lambda(f(x) - f(y)) + f(y)$$

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$\Leftarrow$ For $z = \lambda x + (1-\lambda)y$,

$$\begin{aligned} (*) \quad & f(x) \geq f(z) + \nabla f(z)^{\mathsf{T}}(x-z) \\ (**) \quad & f(y) \geq f(z) + \nabla f(z)^{\mathsf{T}}(y-z). \end{aligned}$$

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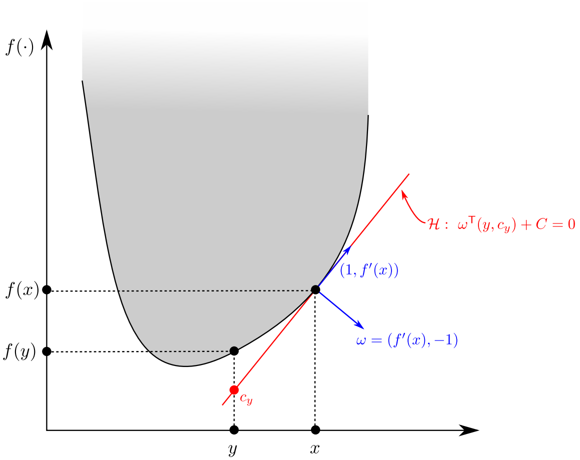
Then $\lambda(*) + (1-\lambda)(**)$ gives

$$\lambda f(x) + (1-\lambda)f(y) \geq f(z) = f(\lambda x + (1-\lambda)y).$$

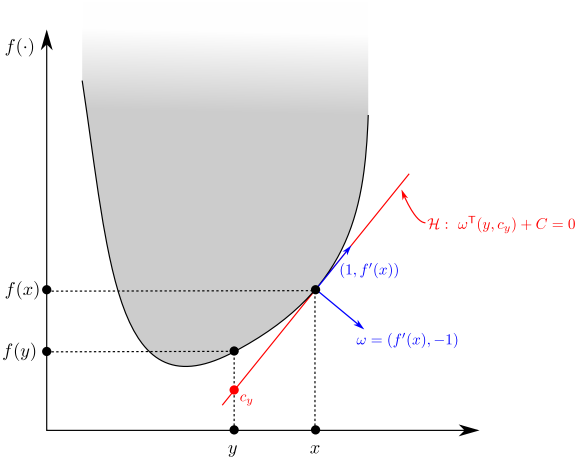
$\square$

Differentiable convex function



Detailed derivation of the first order conditions for $n = 1$:

Differentiable convex function



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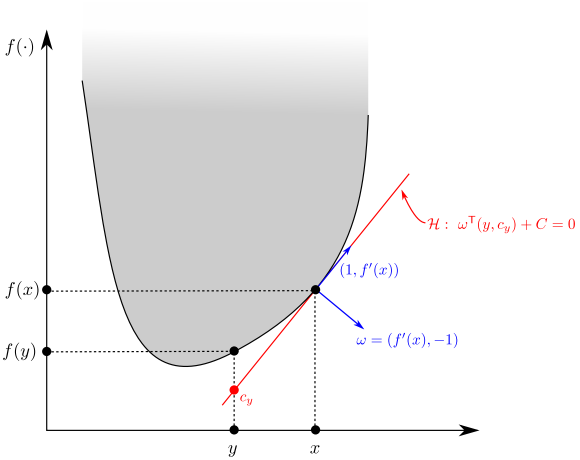

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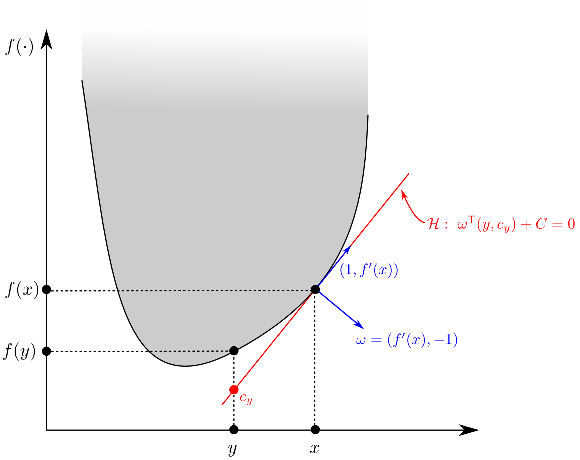

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- using $c_y \leq f(y)$, one retrieves the first order conditions.

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Important consequence: *Fermat's rule*,

Theorem (Fermat's rule)

$x^\star \in \mathcal{X}$ *minimizes* $f : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ *convex iif* $\nabla f(x^\star) = 0$.

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Then, for $h \in \mathcal{X}$ and $\epsilon > 0$,

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True for all h: this implies $\nabla f(x^\star) = 0$.

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so $x^\star$ minimizes f. $\square$

Twice-differentiable convex function

Reminder: For f twice-differentiable at x, Hessian $\nabla^2 f(x) = \{\frac{\partial^2 f}{\partial[x]_i \partial[x]_j}\}_{i,j=1}^n$.

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For $f : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ twice differentiable, f is convex on its domain iif $\nabla^2 f(x)$ is semi-definite positive for all $x \in \mathrm{dom}(f)$.

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For $n = 1$, $\nabla^2 f(x) = f''(x)$.

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Remark (Case $n = 1$)

For $n = 1$, $\nabla^2 f(x) = f''(x)$. Thus, f convex iif $f''(x) > 0$ (or equivalently $f'(x)$ non-decreasing).

Twice-differentiable convex function

Proof.

$\Rightarrow$ By Taylor-Lagrange, $\forall h \in \mathcal{X}$ and $\forall \epsilon > 0$,

$$\exists \gamma \in (0, \epsilon), \; f(x + \epsilon h) = f(x) + \epsilon h^\mathsf{T} \nabla f(x) + \epsilon^2 h^\mathsf{T} \nabla^2 f(x + \gamma h) h$$

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Why? 1D Taylor-Lagrange by differentiating $g : \epsilon \mapsto f(x + \epsilon h)$.

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Using $(1 - t)(*) + t(**)$, we conclude $t f(x) + (1 - t) f(y) \geq g(t) = f(tx + (1 - t)y)$.

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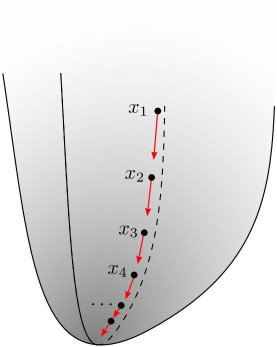
Convex optimization algorithms: descent methods

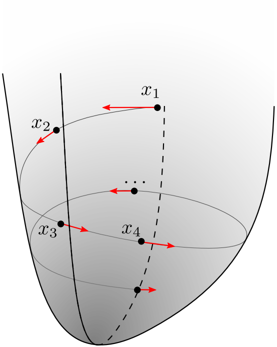
Definition (Descent Method)

Descent method is an algorithm outputing $x_1, x_2, \ldots \in \mathcal{X}$ of the form

$$x_{k+1} = x_k + t_k \Delta x_k, \quad \textit{step size} \quad t_k > 0, \quad \textit{increment} \quad \Delta x_k$$

such that $f(x_{k+1}) < f(x_k)$ if $x_k \notin \operatorname{argmin} f$ and $f(x_{k+1}) = f(x_k)$ if $x_k \in \operatorname{argmin} f$.





Remark (Convergence (or not) of descent algorithms)

For f with non-empty set of minima, descent algorithms converge, however not necessarily to local minimum:

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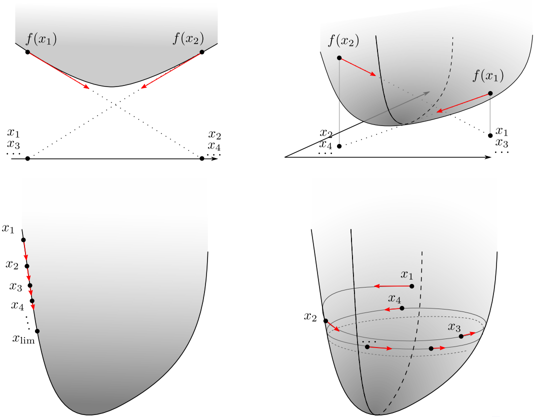
Descent sequences either **not converging** (top) or **not reaching minimum** (bottom).



Convex optimization algorithms: descent methods

Important property: for $x_k, x_{k+1} \in \mathcal{X}$, by first order condition

$$f(x_k + t_k \Delta x_k) \geq f(x_k) + t_k \nabla f(x_k)^{\mathsf{T}} \Delta x_k.$$

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Property (Descent direction)

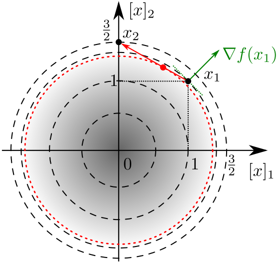
Necessary condition for $x_1, x_2, \ldots$ to be a descent sequence,

$$\nabla f(x_k)^\mathsf{T} \Delta x_k \leq 0$$

where $\Delta x_k = x_{k+1} - x_k$, and equality reached iif $x_k \in \arg\min f$.

Convex optimization algorithms: descent methods

The condition is not sufficient!



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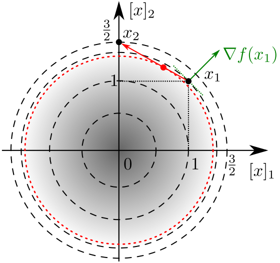

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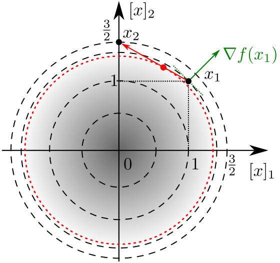

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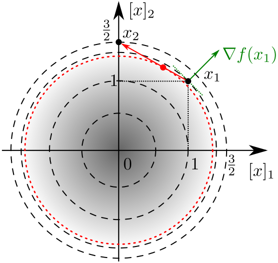

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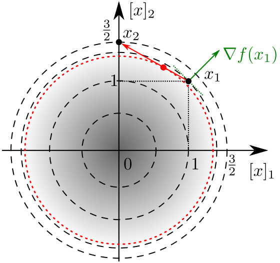

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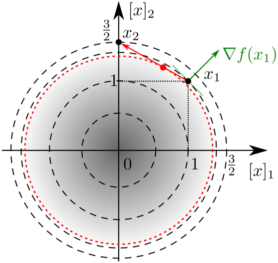

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$\Rightarrow$ **Careful control of step sizes needed!**

Convex optimization algorithms: descent methods

Remark: Still in small step size limit, gain $|f(x_{k+1}) - f(x_k)|$ maximal when $\nabla f(x_k)^\mathsf{T} \Delta x_k$ **both negative and of maximal absolute value**.

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Remark: Often, *constant step*, i.e., $t_k = t$ constant:

- easy: does not request fine-tuning of t_k,
- but suboptimal.

Convex optimization algorithms: descent methods

Definition (Armijo-Goldstein condition)

Given Δx_k with $\|\Delta x_k\| = 1$ and $\nabla f(x_k)^{\mathsf{T}} \Delta x_k < 0$, and $\alpha \in (0, 1)$, t_k satisfies Armijo-Goldstein condition if

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Remark (On step size)

- **[Line search]**

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$$f(x_k + t_k \Delta x_k) < f(x_k) + \alpha t_k \nabla f(x_k)^\mathsf{T} \Delta x_k.$$

Remark: a descent sequence $x_1, x_2, \ldots$.

Remark (On step size)

- **[Line search]**

$$t_k \in \operatorname{argmin}_{t>0} f(x_k + t\Delta x_k)$$

But can be expensive (second optimization or full line search).

Convex optimization algorithms: descent methods

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Convex optimization algorithms: descent methods

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  Always achievable: as $t^{(j)} \to 0$,

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Convex optimization algorithms: convergence of gradient descent

Theorem (Convergence of Gradient Descent with Constant Step Size)

$f : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ *convex, twice continuously differentiable, with L-Lipschitz* ∇f*:*

$$\forall x, y \in \mathcal{X} \qquad \|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|.$$

Then gradient descent with constant step size $t \leq \frac{1}{L}$ *convergences to a minimum of* f*:*

$$x_k \to x^\star \in \operatorname{argmin}_x f(x).$$

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Summing and dividing by ϵ^2:

$$\frac{(\nabla f(x+\epsilon u) - \nabla f(x))^\mathsf{T} u}{\epsilon} = \frac{1}{2} u^\mathsf{T} (\nabla^2 f(x) + \nabla^2 f(x+\epsilon u)) u + o(1).$$

Convex optimization algorithms: convergence of gradient descent

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By Cauchy-Schwarz and the Lipschitz condition,

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Convex optimization algorithms: convergence of gradient descent

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So, as $\epsilon \to 0$,

$$u^{\mathsf{T}} \nabla^2 f(x) u \le L\|u\|^2, \quad \forall u \in \mathcal{X}.$$

$\square$

Convex optimization algorithms: convergence of gradient descent

Proof.

2. Core of Proof. Since f convex $(*)$ and $\nabla^2 f(x) \preceq LI_n$ $(**)$, for $x, y \in \mathcal{X}$,

$$(*)\ f(y) \geq f(x) + \nabla f(x)^{\mathsf{T}}(y-x)$$

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f(x_{k+1}) &\leq f(x_k) + \nabla f(x_k)^{\mathsf{T}}(x_{k+1}-x_k) + \frac{1}{2}L\|x_{k+1}-x_k\|^2 \\
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We now use $t \leq 1/L$:

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f(x_{k+1}) \leq f(x_k) - \frac{t}{2}\|\nabla f(x_k)\|^2 (\leq f(x_k)) \tag{2}
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with equality iif $\nabla f(x_k) = 0$

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with equality iif $\nabla f(x_k) = 0 \Rightarrow$ gradient descent *is* a descent algorithm.

Proof.

3. Convergence to minimum. From $(*)$, for any $x^\star \in \operatorname{argmin} f$ and $x \in \mathcal{X}$,

$$f(x^\star) \geq f(x) + \nabla f(x)^\mathsf{T}(x^\star - x)$$

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which yields

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Convex optimization algorithms: convergence of gradient descent

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Summing for $k = 1, \ldots, K$, RHS *telescopes*:

$$\underbrace{\sum_{k=1}^{K} f(x_{k+1}) - f(x^\star)}_{\geq K(f(x_K) - f(x^\star))} \leq \frac{1}{2t}\left(\|x_1 - x^\star\|^2 - \|x_K - x^\star\|^2\right) \leq \frac{1}{2t}\|x_1 - x^\star\|^2.$$

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So finally, as $K \to \infty$

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Convex optimization algorithms: convergence of gradient descent

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x_K may not converge, but $f(x_K) \to f(x^\star)$. $\square$

Remark (Advantages/limitations of gradient descent)

- *simple to implement*: *for f not easily differentiable, gradient approximation* $\{(f(x_k + \epsilon e_i) - f(x_k))/\epsilon\}_{i=1}^n$ *with* $[e_i]_j = \delta_i^j$ *i-th canonical vector;*

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We can do much better!

Theorem (Linear Convergence of Gradient Descent)

$f : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$ convex, twice continuously differentiable, and $\forall x \in \mathcal{X}$,

$$lI_n \preceq \nabla^2 f(x) \preceq LI_n, \quad \text{for some } L \geq l > 0.$$

Then, ofr gradient descent algorithm with step size $t \leq \frac{1}{L}$,

$$f(x_k) - f(x^\star) \leq \alpha C^k, \quad C < 1.$$

Convex optimization algorithms: convergence speed of gradient descent

Remark: From the proof, convergence speed satisfies at least

$$f(x_k) - f(x^\star) \leq \frac{1}{2kt}\|x_1 - x^\star\|^2.$$

i.e., 100 steps lead to 1% error: **this is quite slow!**, called **sublinear** convergence rate.

We can do much better!

Theorem (Linear Convergence of Gradient Descent)

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Convergence is said **linear**.

Proof.

We already know, since $t \leq \frac{1}{L}$,

$$f(x_{k+1}) \leq f(x_k) - \frac{1}{2} t \|\nabla f(x_k)\|^2$$

Convex optimization algorithms: convergence speed of gradient descent

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Right-hand side minimized for $y = x - \frac{1}{l}\nabla f(x)$ (differentiate along y): $\forall x, y \in \mathcal{X}$,

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Applied to $y = x^\star$ and $x = x_k$,

$$-\frac{t}{2}\|\nabla f(x_k)\|^2 \leq tl(f(x^\star) - f(x_k)).$$

Convex optimization algorithms: convergence speed of gradient descent

Proof.

Back to (3), this implies

$$f(x_{k+1}) - f(x^\star) \leq (1 - tl)\,(f(x_k) - f(x^\star)), \quad 1 - tl = C < 1 \text{ (by assumption)}.$$

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Applied to $k = 1, \ldots, K$, this is

$$f(x_{K+1}) - f(x^\star) \leq C^K (f(x_1) - f(x^\star)).$$

$\square$

Convex optimization algorithms: Newton's method

Intuition of Newton's method: second-order Taylor expansion of f

$$f(x+h) = \underbrace{f(x) + \nabla f(x)^{\mathsf{T}} h + \frac{1}{2} h^{\mathsf{T}} \nabla^2 f(x) h}_{\equiv \hat{f}(x+h)} + o(\|h\|^2).$$

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- approximate $f(x+h)$ by $\hat{f}(x+h)$ for every $x \in \mathcal{X}$
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Definition (Newton's Method)

For f twice-differentiable and $\nabla^2 f(x) \succ 0$ for all $x \in \mathcal{X}$. Then Newton's method:

$$\begin{cases} \Delta x_k & = - \left[\nabla^2 f(x_k)\right] \nabla f(x_k). \\ t_k & = 1 \end{cases}$$

Convex optimization algorithms: Newton's method

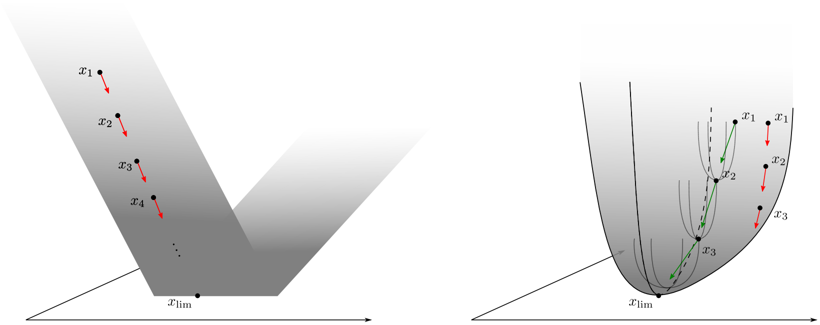

Figure: **(left)** Gradient descent fast on hyperplane-shaped f; **(right)** Newton improves convergence speed, while not following the *steepest descent*.

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- *For* $n \gg 1$*, can be extremely costly (inversion of* $\nabla^2 f(x_k)$ *for every* k*!).*

Convex optimization algorithms: Newton's method

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Definition (Damped Newton's Method)

Damped Newton's method:

$$x_{k+1} = x_k - t_k \left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k)$$

with t_k obtained by *backtracking line search*.

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Theorem (Convergence of damped Newton's method)

Assume $lI_n \preceq \nabla^2 f(x) \preceq LI_n$ and $\nabla^2 f$ is M-Lipschitz, i.e.,

$$\forall x, y, \left\|\nabla^2 f(y) - \nabla^2 f(x)\right\| \leq M\|y - x\|.$$

Then damped Newton's method converges sublinearly then quadratically as soon as $\|\nabla f(x_k)\| < \eta$ for some small $\eta > 0$; besides, from this point on, $t_k = 1$.

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Proof.

First write

$$\begin{aligned}
\|\nabla f(x_{k+1})\| &= \|\nabla f(x_k + \Delta x_k) \underbrace{-\nabla f(x_k) - \nabla^2 f(x_k)\Delta x_k}_{=0}\| \\
&= \left\| \int_0^1 (\nabla^2 f(x_k + u\Delta x_k) - \nabla^2 f(x_k))\Delta x_k du \right\| \\
&\le \frac{M}{2}\|\Delta x_k\|^2 = \frac{M}{2}\|[\nabla^2 f(x_k)]^{-1}\nabla f(x_k)\|^2 \le \frac{M}{2l^2}\|\nabla f(x_k)\|^2.
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Multiplying both sides by $M/(2l^2)$,

$$\frac{M}{2l^2}\|\nabla f(x_K)\| \le \left(\frac{M}{2l^2}\|\nabla f(x_{k_0})\|\right)^2.$$

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Iterated over $k = k_0, \ldots, K$,

$$\|\nabla f(x_K)\| \leq \alpha C^{2^{K-k_0}}$$

with $C = \frac{M}{2l^2}\|\nabla f(x_{k_0})\| < 1$ if $\|\nabla f(x_{k_0})\| < \eta = \frac{2l^2}{M}$. $\square$

Outline

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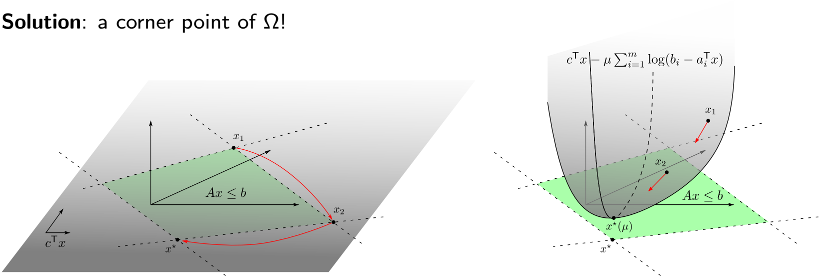

Figure: Linear Programming. **(left)** Simplex method; **(right)** barrier method.

Inequality constrained optimization: the barrier method

Considered problem:

$$\min_{x \in \mathbb{R}^n} f(x) \text{ such that } c_i(x) \geq 0, \; i = 1, \ldots, m$$

where $c_i(x) = a_i^\top x - b_i$ for some $a_i, b_i \in \mathbb{R}^n$.

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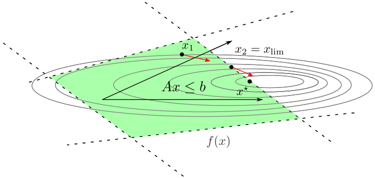

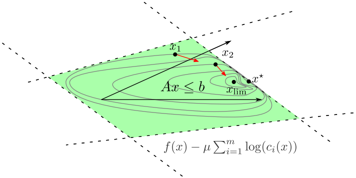

Figure: Barrier Method. **(left)** Level sets of f and constraint set: algorithm "stuck"; **(right)** Level sets of $f - \mu \sum_{i=1}^{m} \log(c_i(x))$ and constraint set: algorithm finds approximation for $x^\star$.

Inequality constrained optimization: the barrier method

Remark (Difficulties of Barrier Method)

Far from ideal...:

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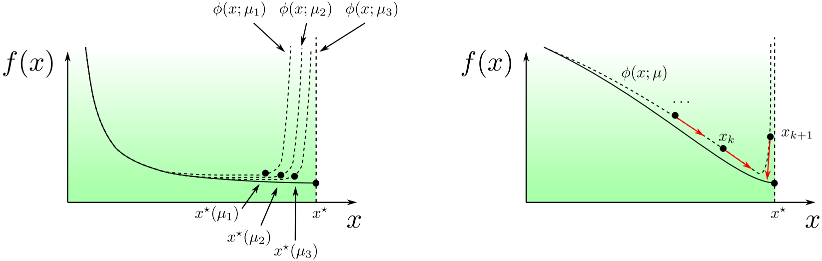

Figure: Barrier Method. **(left)** Sequence of $\phi(x;\mu)$ approx; **(right)** Difficulty raised by sharp minima and "ping-ponging" effect.

Outline

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If $x^\star$ solution to (4), then $\exists \lambda_1, \ldots, \lambda_p \in \mathbb{R}$ such that

$$\nabla f(x^\star) = \sum_{i=1}^{p} (-\lambda_i) \nabla h_i(x^\star).$$

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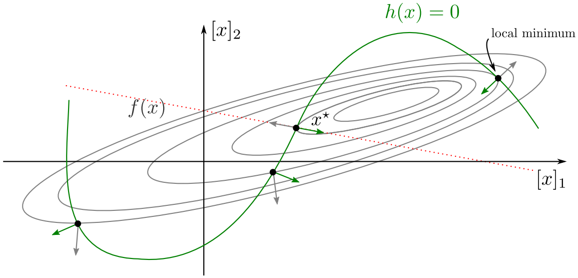

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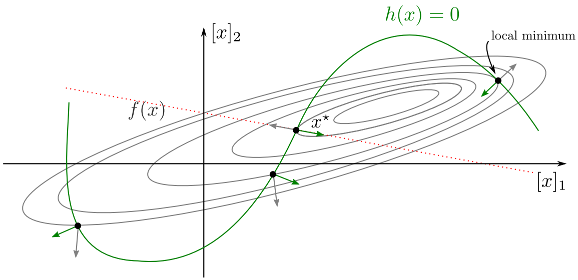

3. When minimum of f coincides with $h(x) = 0$: formula still holds with $\lambda = 0$. □

Linear constraints: Lagrange dual

Consequence: *Necessary condition* for extremum for f under the constraints h_i: find x such that $f(x) + \sum_i \lambda_i h_i(x)$ has zero gradient for some $\lambda_1, \ldots, \lambda_p$.

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For $x^\star$ solution, since $h_i(x^\star) = 0$, we have for all $\lambda \in \mathbb{R}^p$,

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Proof.

For $\lambda_1, \lambda_2 \in \mathbb{R}^p$, $\alpha \in [0, 1]$,

$$\begin{aligned} g(\alpha\lambda_1 + (1-\alpha)\lambda_2) &= \inf_{x \in \mathcal{X}} \left\{ \alpha \left(f(x) + \sum_{i=1}^p \lambda_{1i} h_i(x) \right) + (1-\alpha) \left(f(x) + \sum_{i=1}^p \lambda_{2i} h_i(x) \right) \right\} \\ &\geq \alpha \inf_{x \in \mathcal{X}} \left\{ f(x) + \sum_{i=1}^p \lambda_{1i} h_i(x) \right\} + (1-\alpha) \inf_{x \in \mathcal{X}} \left\{ f(x) + \sum_{i=1}^p \lambda_{2i} h_i(x) \right\} \\ &= \alpha g(\lambda_1) + (1-\alpha) g(\lambda_2) \end{aligned}$$

(inequality follows from $\inf_x\{f_1(x) + f_2(x)\} \geq \inf_x\{f_1(x)\} + \inf_x\{f_2(x)\}$).

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If $\exists x \in \mathcal{X}$ such that $\forall i,\ h_i(x) = 0$ (feasibility), f is convex and h_i affine ($h_i(x) = a_i^\top x + b_i$), then strong duality holds.

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so $g(\lambda^\star) = f(x^\star)$. $\square$

Outline

Equality and inequality constraints

$$\min_{x \in \mathcal{X}} f(x) \text{ such that } g_i(x) \leq 0,\ \ i = 1, \ldots, m \text{ and } h_j(x) = 0,\ j = 1, \ldots, p. \tag{5}$$

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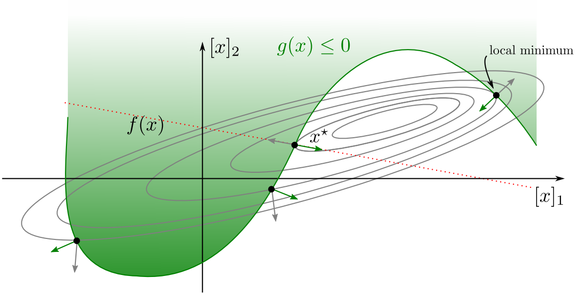

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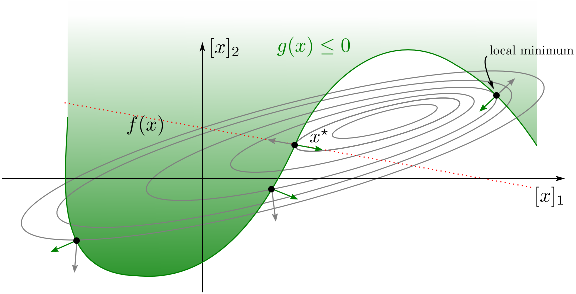

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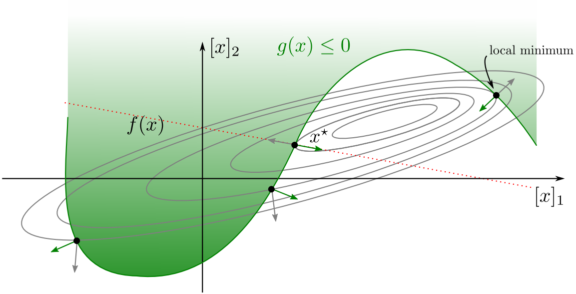

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Lagrange dual of (5) is

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- Hence,

$$x^\star = \arg \min_{\mathcal{X} \cap \left(\bigcap_j \mathcal{G}_j\right) \cap \left(\bigcap_i \mathcal{H}_i\right)} f(x)$$

  i.e., minimising convex f over convex set.

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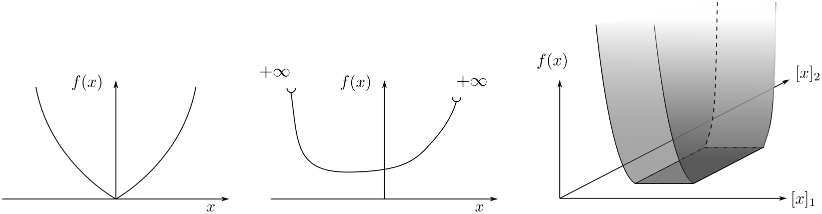

Figure: Examples of not-everywhere differentiable convex functions

Non-differentiable optimization: subgradient

Reminder: first order conditions for convex differentiable $f : \mathcal{X} \to \mathbb{R} \cup \{+\infty\}$,

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Generalization: *subdifferential* of convex f:

Definition (Subdifferential)

Let $f : \mathcal{X} \to \mathbb{R}$. The *subdifferential* ∂f of f is

$$\begin{aligned} \partial f : \mathcal{X} &\to 2^{\mathcal{X}} \\ x &\mapsto \left\{ u \in \mathcal{X} \mid \forall z \in \mathcal{X},\ f(x) \leq f(z) + u^{\mathsf{T}}(x - z) \right\}. \end{aligned}$$

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Let $f : \mathcal{X} \to \mathbb{R}$. The *subdifferential* ∂f of f is

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Non-differentiable optimization: subgradient

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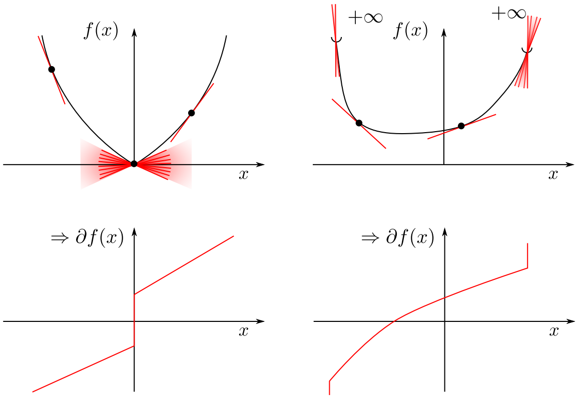
Since f differentiable at x, first order condition gives $\nabla f(x) = u$. □

Non-differentiable optimization: subgradient



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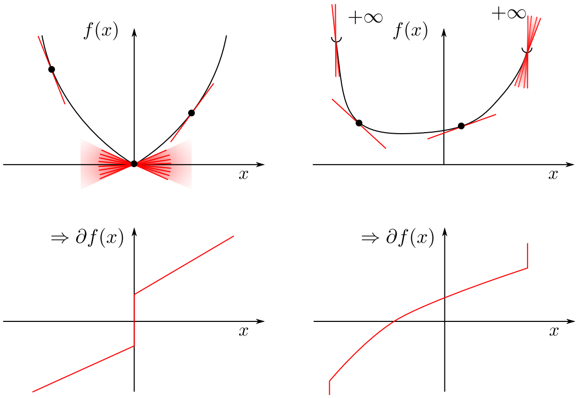

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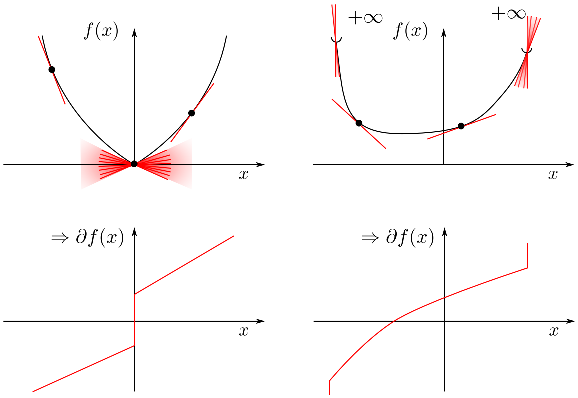

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Property (Subdifferential as union of supporting hyperplanes)

$\partial f(x)$ *consists of the hyperplanes that support* $\mathrm{epi}(f)$ *at* $(x, f(x))$.

Non-differentiable optimization: subgradient

Theorem (Fermat's rule extension)

For $f : \mathcal{X} \to \mathbb{R}$ *convex,*

$$x^\star \in \operatorname{argmin}_{x \in \mathcal{X}} f(x) \Leftrightarrow 0 \in \partial f(x^\star).$$

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Definition (Subgradient algorithm)

Under conditions of gradient descent theorem, with *all Lipschitz subgradients*, subgradient algorithm:

1. $x_{k+1} = x_k - t_k u_k$, for any $u_k \in \partial f(x_k)$
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Remark: 2nd step underlies major weakness of the method (rarely used in practice): algorithm is *not* a descent method.

Outline

From subgradient to proximal

Exercise (The Projection Operator)

For Ω a convex set and $\imath_\Omega$ the set indicator ($\imath_\Omega(x) = 0$ if $x \in \Omega$ and $= +\infty$ if not), define

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- simultaneously (approximately) minimizes objective function, here $\imath_\Omega$.

Non-differentiable optimization: proximal methods

Definition (The Proximal (Point) Operator)

For $f : \mathcal{X} \to \mathbb{R}$ convex, proximal operator prox_f of f is

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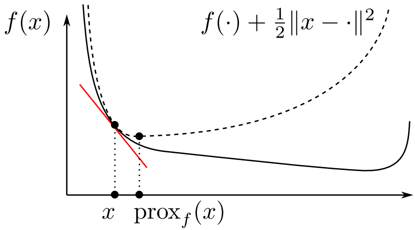

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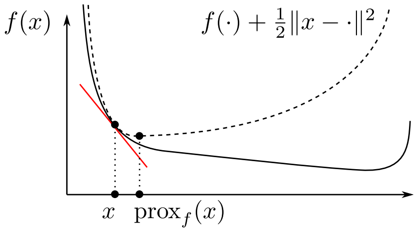

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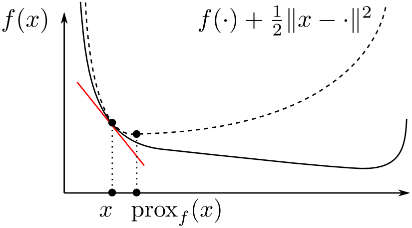

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Operator $D : \mathcal{X} \to 2^{\mathcal{X}}$ is monotone if

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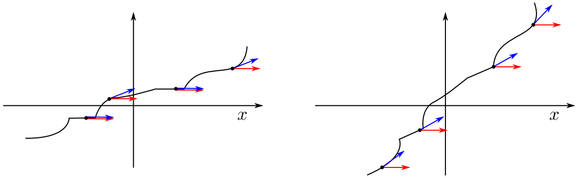

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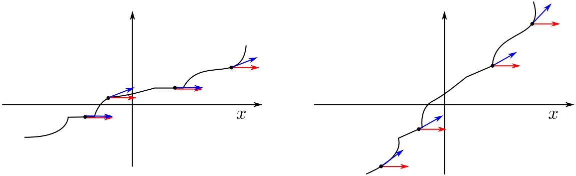

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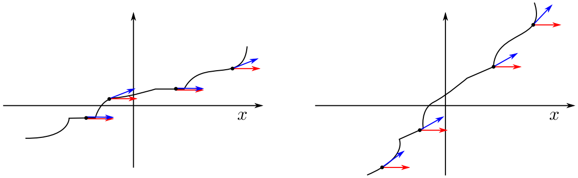

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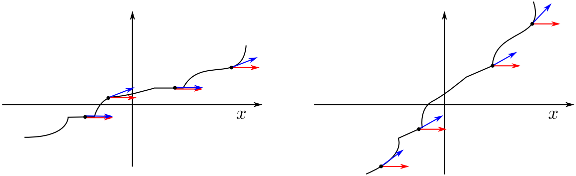

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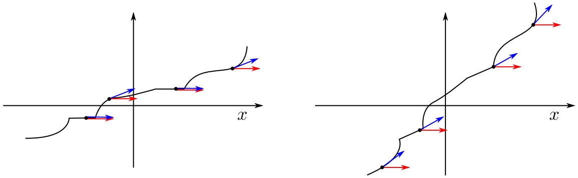

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Non-differentiable optimization: proximal methods

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Consequence. Uniqueness of prox_f makes optimization simpler: f may have multiple minima, $\mathrm{prox}_f(x)$ always unique.

Remark (Properties of prox_f)

For $\lambda > 0$,

$$\mathrm{prox}_{\lambda f}(x) = \underset{y \in \mathcal{X}}{\mathrm{argmin}} \left\{ f(y) + \frac{1}{2\lambda} \|x - y\|^2 \right\}.$$

Non-differentiable optimization: proximal methods

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For $\lambda > 0$,

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Thus, at $y = x$, f and $f + \frac{1}{2\lambda}\|x - \cdot\|^2$ have same value and gradient: prox_f minimizes "local approximation" of f.

Non-differentiable optimization: proximal methods

Key property:

Property (Proximal fixed-points and minimizers)

Minimizers of f are the fixed points of prox_f*:*

$$x^\star \in \operatorname*{argmin}_{x \in \mathcal{X}} f(x) \Leftrightarrow 0 \in \partial f(x^\star) \Leftrightarrow x^\star = \mathrm{prox}_f(x^\star).$$

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Non-differentiable optimization: proximal methods

Definition (Non-expansiveness)

$g : \mathcal{X} \to \mathcal{X}$ *non-expansive* if $\forall x, y \in \mathcal{X}$,

$$\|g(x) - g(y)\| \leq \|x - y\|.$$

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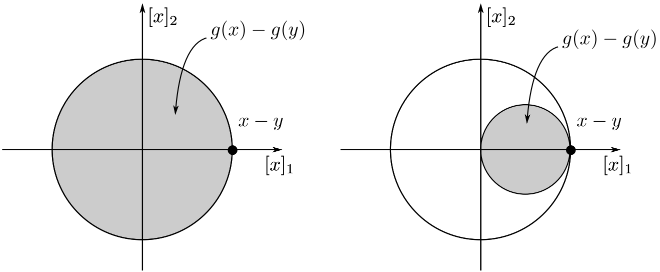

Figure: Non-expansive g (left) and firmly non-expansive g (right).

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Theorem

For convex f, $\mathrm{prox}_f : \mathcal{X} \to \mathcal{X}$, $x \mapsto \mathsf{argmin}_y\, f(y) + \frac{1}{2}\|x - y\|^2$ firmly non-expansive.

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Idea: Prove that $2\mathrm{prox}_f - I$ non-expansive, i.e., $\forall x, y \in \mathcal{X}$,

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For this, recall ∂f is monotone: for $a = \operatorname{prox}_f(x)$ and $b = \operatorname{prox}_f(y)$, then

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Implies

$$(\mathrm{prox}_f(x) - \mathrm{prox}_f(y))^{\mathsf{T}}(x-y) \geq \|\mathrm{prox}_f(x) - \mathrm{prox}_f(y)\|^2 \geq 0 \ .$$

$\square$

Non-differentiable optimization: proximal methods

Main property:

Theorem (The Proximal Point Algorithm)

For $f : \mathcal{X} \to \mathbb{R}$ *convex,* $x_1 \in \mathcal{X}$*, let*

$$x_{k+1} = \mathrm{prox}_f(x_k), \quad \forall k \geq 1.$$

Then $x_k \to x^\star \in \mathrm{argmin}_{x \in \mathcal{X}} \{f(x)\}$.

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Proof.

$$\begin{aligned}
&\|x_{k+1} - x_k\|^2 \\
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&= \|(\mathrm{prox}_f(x_k) - x_k) - (\mathrm{prox}_f(x^\star) - x^\star)\|^2 \\
&= \|\mathrm{prox}_f(x_k) - \mathrm{prox}_f(x^\star)\|^2 + \|x_k - x^\star\|^2 - 2\left(\mathrm{prox}_f(x_k) - \mathrm{prox}_f(x^\star)\right)^{\mathsf{T}}(x_k - x^\star) \\
&\leq \|x_k - x^\star\|^2 - \|\mathrm{prox}_f(x_k) - \mathrm{prox}_f(x^\star)\|^2.
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Last inequality uses *firm non-expansiveness* of prox_f:

$$(\mathrm{prox}_f(x_k) - \mathrm{prox}_f(x^\star))^\mathsf{T}(x_k - x^\star) \geq \|\mathrm{prox}_f(x_k) - \mathrm{prox}_f(x^\star)\|^2 \geq 0 \ .$$

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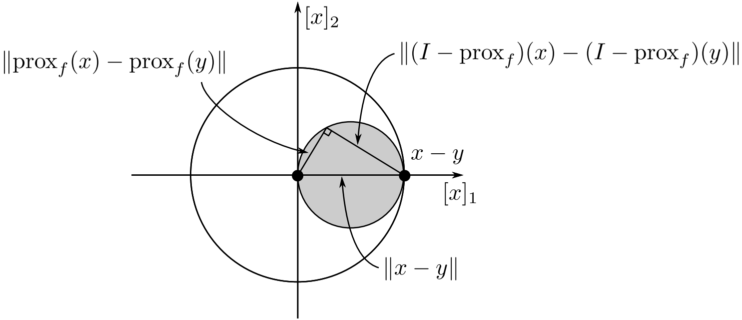
Non-differentiable optimization: proximal methods

Proof.

Geometric interpretation:



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Recall now (non-expansiveness equivalence):

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&\|\mathrm{prox}_f(x) - \mathrm{prox}_f(y)\|^2 - (\mathrm{prox}_f(x) - \mathrm{prox}_f(y))^\mathsf{T}(x-y) \le 0 \\
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Summing over $k = 1, \ldots, K$:

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and thus

$$
\|x_{K+1} - x_K\| \le \frac{1}{\sqrt{K}}\|x_1 - x^\star\| \to 0
$$

as $K \to \infty$, i.e., $\|\mathrm{prox}_f(x_k) - x_k\| \to 0$. $\square$

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Table of classical prox operators:

f	$\mathrm{prox}_f(x)$	$\nabla f(x)$ -
0	x	0
$\imath_\Omega(x)$	$P_\Omega(x)$	-
$\imath_{\mathbb{R}^n_+}(x)$	$\{\max([x]_i, 0)\}_{i=1}^N$	-
$\lambda\|x\|_1$	$\{\mathrm{sgn}([x]_i)\max(\|[x]_i\| - \lambda, 0)\}_{i=1}^n$	-
$\imath_{\{\bar{x}, A\bar{x}=y\}}(x)$	$x + A^\mathsf{T}(AA^\mathsf{T})^{-1}(y - Ax)$	-
$\frac{1}{2}\|Ax - y\|^2$	$(I_n + A^\mathsf{T}A)^{-1}(x + A^\mathsf{T}y)$	$A^\mathsf{T}(Ax - y)$
$x^\mathsf{T}A^\mathsf{T}y$	$x - A^\mathsf{T}y$	$A^\mathsf{T}y$
$\frac{1}{2}x^\mathsf{T}Ax$	$(I_n + A)^{-1}x$	Ax

Outline

Non-differentiable optimization: sum of two functions

Two-function optimization problem: for any convex f_1 and f_2,

$$\min_{x \in \mathcal{X}} f_1(x) + f_2(x)$$

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Case of differentiable convex f_2: with L-Lipschitz gradient ∇f_2 (f_1 *only convex*).

Non-differentiable optimization: sum of two functions

Two-function optimization problem: for any convex f_1 and f_2,

$$\min_{x \in \mathcal{X}} f_1(x) + f_2(x)$$

Crucial example:

- $f_1(x) = \imath_\Omega(x)$ for convex $\Omega \subset \mathcal{X}$
- f_2 any convex function (our previous f).

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Then:

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x^\star \in \operatorname{argmin}_{x \in \mathcal{X}} \{f_1(x) + f_2(x)\} &\Leftrightarrow 0 \in \partial f_1(x^\star) + \nabla f_2(x^\star) \\
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&\Leftrightarrow x^\star \in x^\star + \gamma \partial f_1(x^\star) + \gamma \nabla f_2(x^\star) \\
&\Leftrightarrow x^\star - \gamma \nabla f_2(x^\star) \in x^\star + \gamma \partial f_1(x^\star) \\
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Consequence: equivalent to finding fixed-point for:

$$\mathrm{prox}_{\gamma f_1} \circ (I - \gamma\nabla f_2).$$

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Remark (On parameter γ)

γ *seems artificial.* **But**, *to ensure convergence of fixed-point algorithm,*

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Theorem (Forward-Backward Splitting algorithm)

For $f_1, f_2 : \mathcal{X} \to \mathbb{R}$ *convex with* f_2 *differentiable and with L-Lipschitz gradient, let*

$$\begin{aligned} x_1 &\in \mathcal{X} \\ x_{k+1} &= \mathrm{prox}_{\gamma f_1}\left(x_k - \gamma \nabla f_2(x_k)\right), \quad k \geq 1. \end{aligned}$$

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1. move from x_k to $\tilde{x}_k \equiv x_k - \gamma \nabla f_2(x_k)$, i.e., gradient descent step on f_2 (*forward* progression to minimizing f_2);

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Remark (Forward-Backward Splitting in Practice)

Very convenient in practice to minimize convex differentiable $f = f_2$ under convex constraints given by f_1,

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$$\min_{x \in \Omega} f(x) \quad \Leftrightarrow \quad \min_{x \in \mathcal{X}} \imath_\Omega(x) + f(x)$$

Main advantage: *constrained minimization turned into a much simpler unconstrained minimization of two functions.*

Non-differentiable optimization: sum of two functions

Relaxing differentiable f_2:

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Relaxing differentiable f_2: Proceeding as before, algorithm now iterates

$$(2\mathrm{prox}_{\gamma f_2} - I) \circ (2\mathrm{prox}_{\gamma f_1} - I).$$

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$$\begin{aligned}
&\Leftrightarrow 0 = \mathrm{prox}_{\gamma f_2}(2\tilde{x} - x) - \tilde{x} \\
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Major issue: only *non-expansive* iterations; does not guarantee convergence.

Solution: add extra $\rho \in (0, 1)$ in algorithm steps.

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Theorem (Douglas-Rachford Splitting)

Let $f_1, f_2 : \mathcal{X} \to \mathbb{R}$ *convex. For* $x_0 \in \mathcal{X}$*,* $\lambda > 0$*,* $\rho \in (0,1)$*, and* $k \geq 1$*, let*

$$\begin{aligned} \tilde{x}_k &= \mathrm{prox}_{\gamma f_1}(x_k) \\ x_{k+1} &= x_k + 2\rho \left(\mathrm{prox}_{\gamma f_2}(2\tilde{x}_k - x_k) - \tilde{x}_k \right). \end{aligned}$$

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Then, as $k \to \infty$,

$$x_k \to x^\star \in \mathrm{argmin}_{x \in \mathcal{X}} f_1(x) + f_2(x).$$

The End.