Optimization for Machine Learning

(Problems; Algorithms - A)

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Course materials

- *http://suvrit.de/teaching.html*
- Some references:
  - *Introductory lectures on convex optimization* – Nesterov
  - *Convex optimization* – Boyd & Vandenberghe
  - *Nonlinear programming* – Bertsekas
  - *Convex Analysis* – Rockafellar
  - *Fundamentals of convex analysis* – Urruty, Lemaréchal
  - *Lectures on modern convex optimization* – Nemirovski
  - *Optimization for Machine Learning* – Sra, Nowozin, Wright
  - *Theory of Convex Optimization for Machine Learning* – Bubeck
  - *NIPS 2016 Optimization Tutorial* – Bach, Sra
- Some related courses:
  - EE227A, Spring 2013, (Sra, UC Berkeley)
  - 10-801, Spring 2014 (Sra, CMU)
  - EE364a,b (Boyd, Stanford)
  - EE236b,c (Vandenberghe, UCLA)
- Venues: NIPS, ICML, UAI, AISTATS, SIOPT, Math. Prog.

Lecture Plan

– Introduction (3 lectures)
– Problems and algorithms (5 lectures)
– Non-convex optimization, perspectives (2 lectures)

Constrained problems

Optimality – constrained

♠ For every $x, y \in \operatorname{dom} f$, we have $f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle$.

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- ♠ Thus, x^* is optimal **if** and only if

$$\langle \nabla f(x^*), y - x^* \rangle \geq 0, \qquad \text{for all } y \in \mathcal{X}.$$

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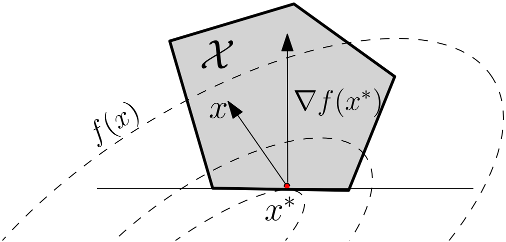
- If $\mathcal{X} = \mathbb{R}^n$, this reduces to $\nabla f(x^*) = 0$



- If $\nabla f(x^*) \neq 0$, it defines supporting hyperplane to $\mathcal{X}$ at x^*

Optimality conditions – constrained

Proof:

- Suppose $\exists y \in \mathcal{X}$ such that $\langle \nabla f(x^*), y - x^* \rangle < 0$
- Using mean-value theorem of calculus, $\exists \xi \in [0, 1]$ s.t.

$$f(x^* + t(y - x^*)) = f(x^*) + \langle \nabla f(x^* + \xi t(y - x^*)), t(y - x^*) \rangle$$

  (we applied MVT to $g(t) := f(x^* + t(y - x^*)))$
- For sufficiently small t, since ∇f continuous, by assump on y, $\langle \nabla f(x^* + \xi t(y - x^*)), y - x^* \rangle < 0$
- This in turn implies that $f(x^* + t(y - x^*)) < f(x^*)$
- Since $\mathcal{X}$ is convex, $x^* + t(y - x^*) \in \mathcal{X}$ is also feasible
- Contradiction to local optimality of x^*

Example: projection operator

$$P_{\mathcal{X}}(z) := \operatorname*{argmin}_{x \in \mathcal{X}} \|x - z\|^2$$

(Assume $\mathcal{X}$ is closed and convex, then projection is unique)
Let $\mathcal{X}$ be nonempty, closed and convex.

- Optimality condition: $x^* = P_{\mathcal{X}}(y)$ iff

$$\langle x^* - z, y - x^* \rangle \geq 0 \text{ for all } y \in \mathcal{X}$$

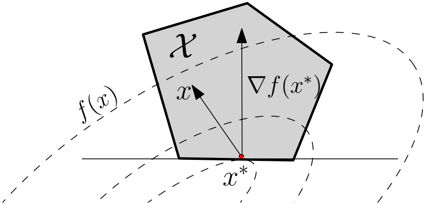
- **Exercise:** Prove that projection is **nonexpansive**, i.e.,

$$\|P_{\mathcal{X}}(x) - P_{\mathcal{X}}(y)\|^2 \leq \|x - y\|^2 \quad \text{for all } x, y \in \mathbb{R}^n.$$

Feasible descent

$$\min \quad f(x) \quad \text{s.t. } x \in \mathcal{X}$$

$$\langle \nabla f(x^*), x - x^* \rangle \geq 0, \qquad \forall x \in \mathcal{X}.$$



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- Stepsize α_k chosen to ensure **feasibility and descent**.

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Since $\mathcal{X}$ is convex, all feasible directions are of the form

$$d^k = \gamma(z - x^k), \quad \gamma > 0,$$

where $z \in \mathcal{X}$ is any feasible vector.

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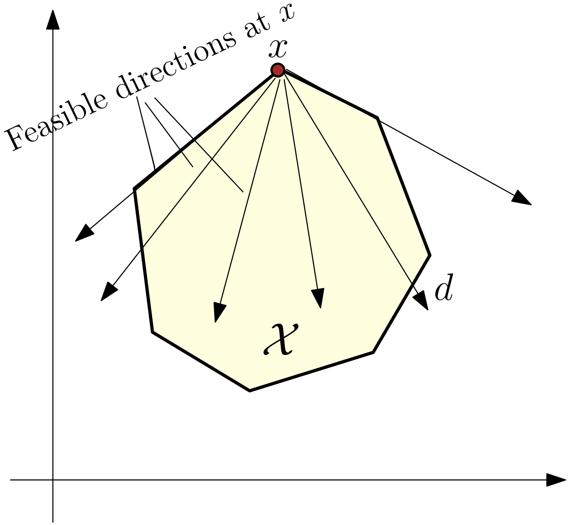
Cone of feasible directions



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Frank-Wolfe (Conditional gradient) method

- Let $z^k \in \text{argmin}_{x \in \mathcal{X}} \langle \nabla f(x^k), x - x^k \rangle$
- Use different methods to select α_k
- $x^{k+1} = x^k + \alpha_k (z^k - x^k)$

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- ♠ Due to M. Frank and P. Wolfe (1956)
- ♠ Practical when solving *linear* problem over $\mathcal{X}$ easy
- ♠ Very popular in machine learning over recent years
- ♠ Refinements, several variants (including nonconvex)

Frank-Wolfe: Convergence

Assum: There is a $C \geq 0$ s.t. for all $x, z \in \mathcal{X}$ and $\alpha \in (0, 1)$:

$$f\big((1-\alpha)x + \alpha z\big) \leq f(x) + \alpha\langle \nabla f(x),\, z - x\rangle + \tfrac{1}{2}C\alpha^2.$$

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A simple induction (**Verify!**) then shows that

$$f(x^k) - f(x^*) \leq \frac{2C}{k+2}, \qquad k \geq 0.$$

Example: Linear Oracle

Suppose $\mathcal{X} = \{\|x\|_p \leq 1\}$, for $p > 1$.

Write Linear Oracle (LO) as maximization problem:

$$\max_z \quad \langle g, z \rangle \quad \text{s.t.} \;\; \|z\|_p \leq 1.$$

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- can be shown that $\|G\|_2$ is the dual norm here.
- Optimal Z satisfies $\langle G, Z\rangle = \|G\|_2 \|Z\|_* = \|G\|_2$; use Lanczos (or using power method) to compute top singular vectors.

(for more examples: Jaggi, Revisiting Frank-Wolfe: ...)

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▶ Linear convergence under quite strong assumptions on both f and $\mathcal{X}$; alternatively, use a more complicated method: *FW with Away Steps* (Guelat-Marcotte 1986); more recently (Jaggi, Lacoste-Julien 2016)

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Projected Gradient

$$x^{k+1} = P_{\mathcal{X}}\big(x^k - \alpha_k \nabla f(x^k)\big), \quad k = 0, 1, \ldots$$

where $P_{\mathcal{X}}$ denotes above orthogonal projection.

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- PG can be much faster than $O(1/k)$ of FW (e.g., $O(e^{-k})$ for strongly convex); but LO can be sometimes much faster than projections.

Projected Gradient – convergence

Depends on the following crucial properties of P:

Nonexpansivity: $\|Px - Py\|_2 \leq \|x - y\|_2$

Firm nonxpansivity: $\|Px - Py\|_2^2 \leq \langle Px - Py,\, x - y\rangle$

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▶ Using projections, essentially convergence analysis with $\alpha_k = 1/L$ for the unconstrained case works.

Exercise: Let $f(x) = \frac{1}{2}\|Ax - b\|_2^2$. Write a Matlab/Python script to minimize this function over the convex set $\mathcal{X} := \{-1 \leq x_i \leq 1\}$ using projected gradient as well as Frank-Wolfe. Compare the two.

Duality

Primal problem

Let $f_i : \mathbb{R}^n \to \mathbb{R}$ $(0 \le i \le m)$. Generic **nonlinear program**

$$\begin{aligned} \min \quad & f_0(x) \\ \text{s.t.}\ & f_i(x) \le 0, \quad 1 \le i \le m, \\ & x \in \{\operatorname{dom} f_0 \cap \operatorname{dom} f_1 \cdots \cap \operatorname{dom} f_m\}. \end{aligned} \tag{P}$$

Def. Domain: The set $\mathcal{D} := \{\operatorname{dom} f_0 \cap \operatorname{dom} f_1 \cdots \cap \operatorname{dom} f_m\}$

- We call (P) the **primal problem**
- The variable x is the **primal variable**
- We will attach to (P) a **dual problem**
- In our initial derivation: no restriction to convexity.

Lagrangian

To the primal problem, associate **Lagrangian** $\mathcal{L} : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$,

$$\mathcal{L}(x, \lambda) := f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x).$$

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- If x is feasible, $\lambda \geq 0$, then we get the lower-bound

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- Lagrangian helps write problem in **unconstrained form**

Lagrangian

Claim: Since, $f_0(x) \geq \mathcal{L}(x, \lambda) \quad \forall x \in \mathcal{X}, \quad \lambda \in \mathbb{R}^m_+$, primal optimal

$$p^* = \inf_{x \in \mathcal{X}} \sup_{\lambda \geq 0} \quad \mathcal{L}(x, \lambda).$$

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- ♠ If x is not feasible, then some $f_i(x) > 0$
- ♠ In this case, inner sup is $+\infty$, so claim true by definition
- ♠ If x is feasible, each $f_i(x) \leq 0$, so $\sup_\lambda \sum_i \lambda_i f_i(x) = 0$

Lagrange dual function

Def. We define the **Lagrangian dual** as

$$g(\lambda) := \inf_x \quad \mathcal{L}(x, \lambda).$$

Lagrange dual function

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$$g(\lambda) := \inf_x \quad \mathcal{L}(x, \lambda).$$

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Observations:

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- Thus, g is concave; it may take value $-\infty$
- Recall: $f_0(x) \geq \mathcal{L}(x, \lambda) \quad \forall x \in \mathcal{X}, \lambda \geq 0$; thus
- $\forall x \in \mathcal{X}, \quad f_0(x) \geq \inf_{x'} \mathcal{L}(x', \lambda) =: g(\lambda)$
- Now minimize over x on lhs, to obtain

$$\forall\, \lambda \in \mathbb{R}^m_+ \qquad p^* \geq g(\lambda).$$

Lagrange dual problem

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- **dual feasible:** if $\lambda \geq 0$ and $g(\lambda) > -\infty$
- **dual optimal:** λ^* if sup is achieved
- Lagrange dual is **always concave**, regardless of original

Weak duality

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$$d^* := \sup_{\lambda \geq 0} \quad g(\lambda).$$

Theorem. (Weak-duality): For problem (P), we have $p^* \geq d^*$.

Proof: We showed that for all $\lambda \in \mathbb{R}^m_+$, $p^* \geq g(\lambda)$.
Thus, it follows that $p^* \geq \sup g(\lambda) = d^*$.

Duality gap

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Several **sufficient** conditions known, especially for convex optimization.

"Easy" necessary and sufficient conditions: **unknown**

Example: Slater's sufficient conditions

$$
\begin{aligned}
\min \quad & f_0(x) \\
\text{s.t.} \quad & f_i(x) \le 0, \quad 1 \le i \le m, \\
& Ax = b.
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Constraint qualification: There exists $x \in \operatorname{ri} \mathcal{D}$ s.t.

$$f_i(x) < 0, \qquad Ax = b.$$

That is, there is a **strictly feasible** point.

> **Theorem.** Let the primal problem be convex. If there is a feasible point such that is strictly feasible for the non-affine constraints (and merely feasible for affine, linear ones), then strong duality holds. Moreover, the dual optimal is attained (i.e., $d^* > -\infty$).

Reading: Read BV §5.3.2 for a proof.

Example: failure of strong duality

$$\min_{x,y} e^{-x} \quad x^2/y \leq 0,$$

over the domain $\mathcal{D} = \{(x, y) \mid y > 0\}$.

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$$\mathcal{L}(x,y,\lambda) = e^{-x} + \lambda x^2/y,$$

so dual function is

$$g(\lambda) = \inf_{x,y>0} e^{-x} + \lambda x^2 y = \begin{cases} 0 & \lambda \geq 0 \\ -\infty & \lambda < 0. \end{cases}$$

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Dual problem

$$d^* = \max_{\lambda} 0 \qquad \text{s.t. } \lambda \geq 0.$$

Thus, $d^* = 0$, and gap is $p^* - d^* = 1$.
Here, we had no strictly feasible solution.

Zero duality gap: nonconvex example

Trust region subproblem (TRS)

$$\min \quad x^T A x + 2b^T x \qquad x^T x \leq 1.$$

A is symmetric but not necessarily semidefinite!

Theorem. TRS always has zero duality gap.

Remark: Above theorem extremely important; part of family of related results for certain quadratic nonconvex problems.

Example: Maxent

$$\begin{aligned} \min \quad & \sum\nolimits_i x_i \log x_i \\ & Ax \leq b, \quad 1^T x = 1, \quad x > 0. \end{aligned}$$

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$$\max_{\lambda,\nu} \quad g(\lambda, \nu) = -b^T\lambda - v - \sum_{i=1}^n e^{-(A^T\lambda)_i - \nu - 1}$$
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If there is $x > 0$ with $Ax \leq b$ and $1^T x = 1$, strong duality holds.
Exercise: Simplify above dual by optimizing out ν

Example: dual for Support Vector Machine

$$\begin{aligned} \min_{x,\xi} \quad & \tfrac{1}{2}\|x\|_2^2 + C\sum_i \xi_i \\ \text{s.t.} \quad & Ax \geq 1 - \xi, \quad \xi \geq 0. \end{aligned}$$

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$$L(x, \xi, \lambda, \nu) = \tfrac{1}{2}\|x\|_2^2 + C1^T\xi - \lambda^T(Ax - 1 + \xi) - \nu^T\xi$$

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$$\begin{aligned} g(\lambda,\nu) &:= \inf L(x,\xi,\lambda,\nu) \\ &= \begin{cases} \lambda^T 1 - \tfrac{1}{2}\|A^T\lambda\|_2^2 & \lambda + \nu = C\mathbf{1} \\ +\infty & \text{otherwise} \end{cases} \\ d^* &= \max_{\lambda \geq 0, \nu \geq 0} \quad g(\lambda,\nu) \end{aligned}$$

Exercise: Using $\nu \geq 0$, eliminate ν from above problem.

Dual via Fenchel conjugates

$$\min f(x) \quad \text{s.t.} \quad f_i(x) \leq 0, \;\; Ax = b.$$

$$\mathcal{L}(x, \lambda, \nu) \quad := \quad f_0(x) + \sum\nolimits_i \lambda_i f_i(x) + \nu^T(Ax - b)$$

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g(\lambda,\nu) &= -\nu^T b - F^*(-A^T\nu).
\end{aligned}$$

Not so useful! F^* hard to compute.

Example: norm regularized problems

$$\min \quad f(x) + \|Ax\|$$

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Say $\|\bar{y}\|_* < 1$, such that $A^T\bar{y} \in \mathrm{ri}(\mathrm{dom} f^*)$, then we have strong duality (e.g., for instance $0 \in \mathrm{ri}(\mathrm{dom} f^*)$)

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Saddle-point formulation

$$p^* \quad = \quad \min_x \max_{u,v} \left\{u^T(b - Ax) + v^T x \mid \|u\|_2 \leq 1, \ \ \|v\|_\infty \leq \lambda\right\}$$

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Example: KKT conditions

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But $\lambda_i^* \geq 0$ and $f_i(x^*) \leq 0$, so **complementary slackness**

$$\lambda_i^* f_i(x^*) = 0, \quad i = 1, \ldots, m.$$

KKT conditions

$$
\begin{aligned}
f_i(x^*) &\leq 0, \quad i = 1, \ldots, m && \text{(primal feasibility)} \\
\lambda_i^* &\geq 0, \quad i = 1, \ldots, m && \text{(dual feasibility)} \\
\lambda_i^* f_i(x^*) &= 0, \quad i = 1, \ldots, m && \text{(compl. slackness)} \\
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- We showed: if strong duality holds, and (x^*, λ^*) exist, then KKT conditions are **necessary** for pair (x^*, λ^*) to be optimal

KKT conditions

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Exercise: Prove the above sufficiency of KKT. *Hint:* Use that $\mathcal{L}(x, \lambda^*)$ is convex, and conclude from KKT conditions that $g(\lambda^*) = f_0(x^*)$, so that (x^*, λ^*) optimal primal-dual pair.