Optimization for Machine Learning

Lecture 4: Optimality conditions

6.881: MIT

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Optimality

(Local and global optima)

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- So rhs is also nonnegative, proving $f(y) \geq f(x^*)$ as desired.

Set of Optimal Solutions

The set of optimal solutions $\mathcal{X}^*$ may be empty

Example. If $\mathcal{X} = \emptyset$, i.e., no feasible solutions, then $\mathcal{X}^* = \emptyset$

Example. When only inf not min, e.g., $\inf e^x$ as $x \to -\infty$
in general, we should worry about the question "Is $\mathcal{X}^* = \emptyset$?"

Exercise: Verify that $\mathcal{X}^*$ is always a convex set.

Optimality conditions

(Recognizing optima)

First-order conditions: unconstrained

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Exercise: Prove that if f is convex, then $\nabla f(x^*) = 0$ is actually **sufficient** for global optimality! For general f this is ***not*** true. (This property is what makes convex optimization special!)

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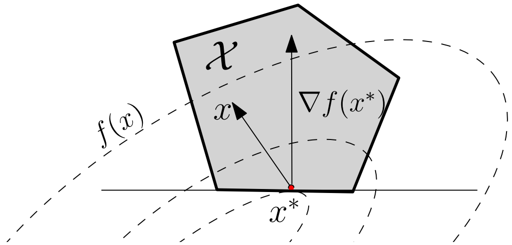
- If $\mathcal{X} = \mathbb{R}^n$, this reduces to $\nabla f(x^*) = 0$



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

First-order conditions: constrained

- Let f be continuously differentiable, possibly nonconvex
- 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^*

Optimality without differentiability

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Nonsmooth problem

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

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Observe: If constraint satisfied strictly at optimum ($\|x\| < 1$), then $\nabla f(x) = 0$ (else we'd violate the last inequality above).

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(KKT and friends)

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Thus, there exists a pair (x^*, λ^*) such that

$p^* = f(x^*)$

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Assume strong duality and that p^*, d^* attained!

Thus, there exists a pair (x^*, λ^*) such that

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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

Karush-Kuhn-Tucker Conditions (KKT)

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\begin{array}{rcll}
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)} \\
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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.

Read Ch. 5 of BV

Examples

Projection onto a hyperplane

$$\min_x \ \tfrac{1}{2}\|x - y\|^2, \quad \text{s.t.} \ \ a^T x = b.$$

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$$\begin{aligned} L(x,\nu) &= \tfrac{1}{2}\|x-y\|^2 + \nu(a^T x - b) \\ \frac{\partial L}{\partial x} &= x - y + \nu a = 0 \end{aligned}$$

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Projection onto a hyperplane

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$$\boxed{x = y - \tfrac{1}{\|a\|^2}(a^T y - b)a}$$

Projection onto simplex

$$\min_x \ \tfrac{1}{2}\|x - y\|^2, \quad \text{s.t.} \quad x^T 1 = 1, x \geq 0.$$

KKT Conditions

$$L(x, \lambda, \nu) \qquad = \tfrac{1}{2}\|x - y\|^2 - \sum\nolimits_i \lambda_i x_i + \nu(x^T 1 - 1)$$

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Challenge A. Solve the above conditions in $O(n \log n)$ time.

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Total variation minimization

$$\min \quad \tfrac{1}{2}\|x-y\|^2 + \lambda \sum_i |x_{i+1} - x_i|,$$

$$\min \quad \tfrac{1}{2}\|x-y\|^2 + \lambda\|Dx\|_1,$$

(the matrix D is also known as a differencing matrix).

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Step 1. Take the dual (recall from L3-25) to obtain:

$$\min_u \tfrac{1}{2}\|D^T u\|^2 - u^T D y, \quad \text{s.t.} \quad \|u\|_\infty \le \lambda.$$

Step 2. Replace obj by $\|D^T u - y\|^2$ (argmin is unchanged)

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Step 4 (Challenge). Look at KKT conditions, and keep working …finally, obtain $O(n)$ method!
For full-story look at: *A. Barbero, S. Sra. "Modular proximal optimization for multidimensional total-variation regularization" (JMLR 2019, pp. 1–82)*

Nonsmooth KKT

(via subdifferentials)

KKT via subdifferentials*

Assume all $f_i(x)$ are finite valued, and $\operatorname{dom} f = \mathbb{R}^n$

$$\min_{x\in\mathbb{R}^n} f(x) \quad \text{s.t.} \;\; f_i(x) \leq 0, \;\; i \in [m].$$

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Write $C_i := \{x \mid f_i(x) \leq 0\}$. Then, above problem becomes

$$\min_{x} \quad \phi(x) := f(x) + \mathbb{1}_{C_1}(x) + \cdots + \mathbb{1}_{C_m}(x).$$

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An optimal solution to this problem is a vector $\bar{x}$ such that

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Slater's condition tells us that

$$\operatorname{int} C_1 \cap \cdots \cap \operatorname{int} C_m \neq \emptyset.$$

Exercise: Rigorously justify the above (*Hint:* use continuity of f_i)

KKT via subdifferentials*

Since $\operatorname{int} C_1 \cap \cdots \cap \operatorname{int} C_m \neq \emptyset$, Rockafellar's theorem tells us

$$\partial\phi(x) = \partial f(x) + \partial \mathbb{1}_{C_1}(x) + \cdots + \partial \mathbb{1}_{C_m}(x).$$

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Recall: $\partial \mathbb{1}_{C_i} = \mathcal{N}_{C_i}$ (normal cone). **Verify (Challenge)** that

$$\mathcal{N}_{C_i}(x) = \begin{cases} \bigcup \{\lambda_i \partial f_i(x) \mid \lambda_i \geq 0\}, & \text{if } f_i(x) = 0, \\ \{0\}, & \text{if } f_i(x) < 0, \\ \emptyset, & \text{if } f_i(x) > 0. \end{cases}$$

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Thus, $\partial\phi(x) \neq \emptyset$ iff x satisfies $f_i(x) \leq 0$
(**Verify:** that the Minkowski sum $A + \emptyset = \emptyset$)

KKT via subdifferentials*

Thus, $\partial\phi(x) = \bigcup\{\partial f(x) + \lambda_1 \partial f_1(x) + \cdots + \lambda_m \partial f_m(x)\}$, *over all choices* of $\lambda_i \geq 0$ such that

$$\lambda_i f_i(x) = 0.$$

If $f_i(x) < 0$, $\partial\mathbb{1}_{C_i} = \{0\}$, while for $f_i(x) = 0$, $\partial\mathbb{1}_{C_i}(x) = \{\lambda_i \partial f_i(x) \mid \lambda_i \geq 0\}$, and we cannot jointly have $\lambda_i \geq 0$ and $f_i(x) > 0$.

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In other words, $0 \in \partial\phi(x)$ **iff** there exist $\lambda_1, \ldots, \lambda_m$ that satisfy the KKT conditions.

Exercise: Double check the above for differentiable f, f_i

Example: Constrained regression

$$\min_x \ \tfrac{1}{2}\|Ax - b\|^2, \quad \text{s.t. } \|x\| \leq \theta.$$

KKT Conditions

$$\begin{aligned}
L(x, \lambda) &= \tfrac{1}{2}\|Ax - b\|^2 + \lambda(\|x\| - \theta) \\
0 &\in A^T(Ax - b) + \lambda \partial\|x\| \\
\partial\|x\| &= \begin{cases} \|x\|^{-1}x & x \neq 0, \\ \{z \mid \|z\| \leq 1\} & x = 0. \end{cases}
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Hmmm...?

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- *Case (i).* $x \leftarrow \texttt{pinv}(A)b$ and $\|x\| < \theta$, then $x^* = x$
- *Case (ii).* If $\|x\| \ge \theta$, then $\|x^*\| = \theta$. Thus, consider instead $\frac{1}{2}\|Ax-b\|^2$ s.t. $\|x\|^2 = \theta^2$. (**Exercise:** complete the idea.)