CME 307 / MS&E 311: Optimization Optimality conditions and convexity

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Questions from last class

- clarify proof of strong duality
- how many iterations of branch and bound?
- how to use duality to solve a problem? when to stop?
- duality for problems with inequality constraints?

Outline

Constrained and unconstrained optimization

Optimality conditions

Convex optimization

Constrained vs unconstrained optimization

constrained optimization

- examples: scheduling, routing, packing, logistics, scheduling, control
- what's hard: finding a feasible point

unconstrained optimization

- examples: data fitting, statistical/machine learning
- what's hard: reducing the objective

both are necessary for real-world problems!

Unconstrained smooth optimization

for $f: \mathbf{R}^n \to \mathbf{R}$ ctsly differentiable,

minimize
$$f(x)$$
 variable $x \in \mathbf{R}^n$

how to solve?

Unconstrained smooth optimization

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how to solve? approximate as a quadratic problem

$$f(x) \approx f(x_0) + \nabla f(x_0)^T (x - x_0) + \frac{1}{2} (x - x_0)^T H(x_0) (x - x_0)$$

and find solution x_{quad} to the quadratic problem. then set $x_0 \leftarrow x_{\text{quad}}$ and repeat.

Nonlinear optimization

optimization problem: nonlinear form

minimize
$$f_0(x)$$

subject to $f_i(x) \leq b_i, \quad i = 1, \dots, m_1$
 $h(x) = 0$
variable $x \in \mathbf{R}^n$

- \triangleright $x = (x_1, \dots, x_n)$: optimization variables
- ▶ $f_0 : \mathbf{R}^n \to \mathbf{R}$: objective function
- ▶ $f_i : \mathbf{R}^n \to \mathbf{R}$, i = 1, ..., m: constraint functions

special case: unconstrained optimization

Example: process control

You are the process engineer for a desalination plant that produces drinking water. The plant has a variety of knobs, collected in vector x, that you can turn to control the process. These control, e.g., how much water is pumped into the plant, how much pressure is used to force the water through filters, and how much of each chemical is added to the water.

- $ightharpoonup f_0(x)$: cost of water produced
- $ightharpoonup f_i(x)$: level of each measured impurity in the water
- ▶ b_i: maximum allowable level of each impurity

Given a setting of the knobs, you can observe the cost of water produced and the levels of impurities.

What is the optimal setting of the knobs?

Oracles

an optimization **oracle** is your interface for accessing the problem data:

e.g., an oracle for $f: \mathbf{R}^n \to \mathbf{R}$ can evaluate for any $x \in \mathbf{R}^n$:

- ightharpoonup zero-order: $f_0(x)$
- ▶ **first-order:** $f_0(x)$ and $\nabla f_0(x)$
- **second-order:** $f_0(x)$, $\nabla f_0(x)$, and $\nabla^2 f_0(x)$

why oracles?

- can optimize real systems based on observed output (not just models)
- can use and extend old or complex but trusted code (e.g., NASA, PDE simulations, ...)
- can prove lower bounds on the oracle complexity of a problem class

source: Nesterov 2004 "Introductory Lectures on Convex Optimization"

Nonlinear optimization: how to solve?

depends on the oracle:

- first- or second-order: approximate by a sequence of quadratic problems
- zero-order: harder, lots of methods
 - simulated annealing
 - Bayesian optimization
 - pseudo-higher-order methods, e.g., compute approximate gradient

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Solution of an optimization problem

minimize
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for $f: \mathcal{D} \to \mathbf{R}$. x^* is a

- **proof** global minimizer if $f(x) \ge f(x^*)$ for all $x \in \mathcal{D}$.
- ▶ **local minimizer** if there is a neighborhood \mathcal{N} around x^* so that $f(x) \geq f(x^*)$ for all $x \in \mathcal{N}$.
- **isolated local minimizer** if the neighborhood $\mathcal N$ contains no other local minimizers.
- unique minimizer if it is the only global minimizer.

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pictures!

First order optimality condition

Theorem

If $x^* \in \mathbb{R}^n$ is a local minimizer of a differentiable function $f : \mathbb{R}^n \to \mathbb{R}$, then $\nabla f(x^*) = 0$.

First order optimality condition

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If $x^* \in \mathbb{R}^n$ is a local minimizer of a differentiable function $f : \mathbb{R}^n \to \mathbb{R}$, then $\nabla f(x^*) = 0$.

proof: suppose by contradiction that $\nabla f(x^*) \neq 0$. consider points of the form $x_{\alpha} = x^* - \alpha \nabla f(x^*)$ for $\alpha > 0$. by definition of the gradient,

$$\lim_{\alpha \to 0} \frac{f(x_{\alpha}) - f(x^{\star})}{\alpha} = -\nabla f(x^{\star})^{\top} \nabla f(x^{\star}) = -\|\nabla f(x^{\star})\|^{2} < 0$$

so for any sufficiently small $\alpha > 0$, we have $f(x_{\alpha}) < f(x^{*})$, which contradicts the fact that x^{*} is a local minimizer.

Second order optimality condition

Theorem

If $x^* \in \mathbb{R}^n$ is a local minimizer of a twice differentiable function $f: \mathbb{R}^n \to \mathbb{R}$, then $\nabla^2 f(x^*) \succeq 0$.

Second order optimality condition

Theorem

If $x^* \in \mathbf{R}^n$ is a local minimizer of a twice differentiable function $f: \mathbf{R}^n \to \mathbf{R}$, then $\nabla^2 f(x^*) \succeq 0$.

proof: similar to the previous proof. use the fact that the second order approximation

$$f(x_{\alpha}) \approx f(x^{\star}) + \nabla f(x^{\star})^{\top} (x_{\alpha} - x^{\star}) + \frac{1}{2} (x_{\alpha} - x^{\star})^{\top} \nabla^{2} f(x^{\star}) (x_{\alpha} - x^{\star})$$

is accurate locally to show a contradiction unless $\nabla^2 f(x^*) \succeq 0$: if not, there is a direction v such that $v^T \nabla^2 f(x^*) v < 0$. then $f(x + \alpha v) < f(x^*)$ for α arbitrarily small, which contradicts the fact that x^* is a local minimizer.

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A set $S \subseteq \mathbb{R}^n$ is convex if it contains every chord: for all $\theta \in [0,1]$, w, $v \in S$,

$$\theta w + (1 - \theta)v \in S$$

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Q: Which of these are convex? ellipsoid, half moon

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► **Second order condition.** If *f* is twice differentiable, its Hessian is always psd:

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Q: Which of these are convex? quadratic, abs, pwl, step, jump, logistic, logistic loss

Convex optimization

an optimization problem is convex if:

- ► **Geometrically:** the feasible set and the epigraph of the objective are convex
- ► **NLP:** the objective and inequality constraints are convex functions, and the equality constraints are affine

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- relatively complete theory
- efficient solvers
- conceptual tools that generalize

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- \triangleright a function f is concave if -f is convex
- ▶ concave maximization ⇒ a convex optimization problem

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proof? suppose by contradiction that another point x' is a global minimizer, with $f(x') < f(x^*)$. draw the chord between x' and x^* . since the chord lies above f, every convex combination $x = \theta x^* + (1-\theta)x'$ of x' and x^* for $\theta \in (0,1)$ has a value $f(x) < f(x^*)$. this is true even for $x \to x^*$, contradicting our assumption that x^* is a local minimizer.

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Q: Is a global minimizer of a convex function always unique?

A: No. Picture.

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Q: Can a global minimum have a non-zero gradient?

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A: Yes.

 $\nabla f(x^*) = 0$ is the **first-order (necessary) condition** for optimality.

Invex function

Definition

A function $f: \mathbb{R}^n \to \mathbb{R}$ is **invex** if for some vector-valued function $\eta: \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$,

$$f(x) - f(u) \ge \eta(x, u)^{\top} \nabla f(u)$$
 $\forall u \in \mathbf{R}^n, x \in \operatorname{dom} f$

Theorem (Craven and Glover, Ben-Israel and Mond)

A function is invex iff every stationary point is a global minimum.