CME 307 / MS&E 311: Optimization

Introduction

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Management Science and Engineering
Stanford

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Announcements

- website: https://stanford-cme-307.github.io/web
- Ed for discussion and announcements: https://edstem.org/us/courses/51411/
- fill out course survey (also linked on website): https://forms.gle/7hPniFeC576S12FAA
- talk to me after class and/or schedule office hours (see website)
- class attendance is required. will post some slides, generally no recordings

Intro exercise

Form groups of three people you haven't met before and introduce yourselves.

- name, major, year
- why are you interested in optimization?
- what are you hoping to learn?

Goals for today

- Understand course objectives and expectations
- Identify several types of optimization problem
- Meet at least two other students you've not met before
- Discuss challenges in a real-world optimization problem

Outline

What is an optimization problem?

Course goals and expectations

Exercise

Discuss in groups:

- give an example of a real-world optimization problem
- what is the problem data?
- what are the problem variables?
- how would you write it down?

(Integer) linear optimization problem

$$
\begin{array}{ll}
\text{minimize} & c^T x \\
\text{subject to} & Ax = b \\
& \ell \leq x \leq u \\
\text{variable} & x \in \mathbb{Z}^n
\end{array}
$$

- objective $c^T x$
- equality constraints $Ax = b$
- lower and upper bounds $\ell \leq x \leq u$
- integer variable

problem data:

- $A \in \mathbf{R}^{m \times n}$, $b \in \mathbf{R}^m$
- $c \in \mathbf{R}^n$
- $\ell \in \mathbf{R}^n$, $u \in \mathbf{R}^n$

Nonlinear optimization problem

$$
\begin{array}{ll}
\text{minimize} & f_0(x) \\
\text{subject to} & f_i(x) \leq 0, \quad i = 1, \ldots, m_1 \\
& h_i(x) = 0, \quad i = 1, \ldots, m_2 \\
\text{variable} & x \in \mathbf{R}^n
\end{array}
$$

- objective f_0
- inequality constraints f_i
- equality constraints h_i

problem data:

- (blackbox) code to evaluate f_i and h_i for any $x \in \mathbf{R}^n$
- (first order) and to compute gradients
- (second order) and to compute Hessians

Optimization problems

important optimization problem classes:

- linear
- integer
- nonlinear (with linear or nonlinear constraints)
- quadratic
- unconstrained
- finite-sum
- conic
- convex
- black-box with (0, 1, or 2)-order oracle

Optimization problems

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draw a picture relating these

Discuss

Does your problem fit into one of these categories?

- which?
- if not, why not?

Modularity in optimization

how to optimize:

1. model problem as a mathematical optimization problem
2. identify the properties of the problem
3. use an appropriate solver (or write a new one)

. . . and iterate:

- approximate the problem to make it easier
- solve a sequence of approximated problems that converge to solve the original problem
- or initialize ("warm-start") a solver for the original problem with a solution to the approximated problem

Outline

What is an optimization problem?

Course goals and expectations

Course goals

look at goals on course website: https://stanford-cme-307.github.io/web/

- Which goals sound exciting?
- Which goals don't make sense?
- What else do you hope to accomplish?

Course expectations

look at grading tab on course website: https://stanford-cme-307.github.io/web/
discuss:

- do expectations make sense given course goals?
- questions about expectations?

Course schedule

look at materials tab on course website and at spreadsheet of topics:
https://stanford-cme-307.github.io/web/

Course project

read project expectations and ideas. discuss in groups:

- do you want to work on algorithms, applications, or LLM tools?
- pick a problem. what data would you need? what challenges would you foresee in solving it?

What next?

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Quadratic optimization

Nonlinear optimization

Conic optimization

Integer programming

Convex optimization

Quadratic optimization

a **quadratic optimization** problem is written as

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|Ax - b\|^2 := f_0(x) \\ \text{variable} & x \in \mathbf{R}^n \end{array}$$

where

- $A \in \mathbf{R}^{m \times n}$: matrix
- $b \in \mathbf{R}^m$: vector

how to solve?

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how to solve? take gradient and set to 0:

$$\nabla f_0(x) = A^T(Ax - b) = 0$$

$\Longrightarrow$ linear system solvers also solve quadratic optimization problems

Linear algebra review

matrix $A \in \mathbf{R}^{m \times n}$

- check matrix calculus results by checking dimensions

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  - null space of A, $\mathbf{nullspace}(A)$, is a hyperplane of dimension

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  - null space of A, $\mathbf{nullspace}(A)$, is a hyperplane of dimension $n - m$
  - solution set is $\{x : Ax = b\} = \{x_0 + Vz\}$ where columns of $V \in \mathbf{R}^{n \times n-m}$ span $\mathbf{nullspace}(A)$

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- $A^T A$ is symmetric positive semidefinite (proof on board)

Symmetric positive semidefinite matrices

Definition

a symmetric matrix $Q \in \mathbf{R}^{n\times n}$ is **positive semidefinite** (psd) if $x^T Qx \geq 0$ for all $x \in \mathbf{R}^n$.

these matrices are so important that there are many ways to write them! for $Q \in \mathbf{R}^{n\times n}$,

$$Q \in \mathbf{S}^n_+ \iff Q \succeq 0 \iff Q = Q^T,\ \lambda_{\min}(Q) \geq 0$$

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$Q \in \mathbf{S}_+^n$ is **symmetric positive definite** (spd) ($Q \succ 0$) if $x^T Q x > 0$ for all $x \in \mathbf{R}^n$.

why care about psd matrices Q?

- least-squares objective has a psd $Q = A^T A$
- level sets of $x^T Q x$ are (bounded) ellipsoids
- the quadratic form $x^T Q x$ is a metric iff $Q \succ 0$
- eigenvalue decomp and svd coincide for psd matrices

Quadratic program

a **quadratic program** is written as

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}x^T Qx + c^T x \\ \text{subject to} & Ax = b \\ \text{variable} & x \in \mathbf{R}^n \end{array}$$

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how to solve? reduce to quadratic optimization problem:

- (explicit) form solution set $\{x : Ax = b\} = \{x_0 + Vz \mid z \in \mathbf{R}^{n-m}\}$ by computing a solution $Ax_0 = b$ and a basis V for the null space of A
- (implicit) use duality to recast problem as larger linear (KKT) system

Quadratic program: application

Markowitz portfolio optimization problem:

$$
\begin{array}{ll}
\text{minimize} & \gamma x^T \Sigma x - \mu^T x \\
\text{subject to} & \sum_i x_i = 1 \\
& Ax = 0 \\
\text{variable} & x \in \mathbf{R}^n
\end{array}
$$

where

- $\Sigma \in \mathbf{R}^{n \times n}$: asset covariance matrix
- $\mu \in \mathbf{R}^n$: asset return vector
- $\gamma \in \mathbf{R}$: risk aversion parameter
- rows of $A \in \mathbf{R}^{m \times n}$ correspond to other portfolios
  - ensures new portfolio is independent, *e.g.*, of market returns

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Unconstrained smooth optimization

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

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{variable} & x \in \mathbf{R}^n \end{array}$$

how to solve?

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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.

Finite sum

finite sum optimization problem

$$\begin{array}{ll} \text{minimize} & \sum_{i=1}^m f_i(x) \\ \text{variable} & x \in \mathbf{R}^n \end{array}$$

key fact: can approximate gradient using gradient on **minibatch** $S \subseteq \{1, \ldots, m\}$:

$$\nabla f(x) \approx \frac{1}{|S|} \sum_{i \in S} \nabla f_i(x)$$

examples:

- statistical learning (logistic regression, SVM)
- deep learning

Background: classification

classification problem: m data points

- feature vector $a_i \in \mathbf{R}^n$, $i = 1, \ldots, m$
- label $b_i \in \{-1, 1\}$, $i = 1, \ldots, m$

choose decision boundary $a^T x = 0$ to separate data points into two classes

- $a^T x > 0 \implies$ predict class 1
- $a^T x < 0 \implies$ predict class -1

classification is correct if $b_i a^T x > 0$

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- projective transformation transforms affine boundary to linear boundary
- classification is invariant to scalar multiplication of x

Logistic regression

(regularized) **logistic regression** minimizes the **finite sum**

$$\begin{array}{ll} \text{minimize} & \sum_{i=1}^m \log(1+\exp\left(-b_i a_i^T x\right)) + r(x) \\ \text{variable} & x \in \mathbf{R}^n \end{array}$$

where

- $b_i \in \{-1, 1\}$, $a_i \in \mathbf{R}^n$
- $r : \mathbf{R}^n \to \mathbf{R}$ is a **regularizer**, *e.g.*, $\|x\|^2$ or $\|x\|_1$

Support vector machine

support vector machine (SVM) minimizes the **finite sum**

$$\begin{array}{ll} \text{minimize} & \sum_{i=1}^{m} \max(0, 1 - b_i a_i^T x) + \gamma \|x\|^2 \\ \text{variable} & x \in \mathbf{R}^n \end{array}$$

where $b_i \in \{-1, 1\}$ and $a_i \in \mathbf{R}^n$.

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how to solve?

- use **subgradient** method
- transform to **conic form**
- solve **dual** problem instead
- **smooth** the objective

Nonlinear optimization

optimization problem: nonlinear form

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq b_i, \quad i = 1, \ldots, m_1 \\ & h(x) = 0 \\ \text{variable} & x \in \mathbf{R}^n \end{array}$$

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

- $f_0(x)$: cost of water produced
- $f_i(x)$: 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 $x \in \mathbf{R}^n$:

- **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

Solution of an optimization problem

$$\text{minimize} \quad f(x)$$

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

- **local minimizer** if there is a neighborhood $\mathcal{N}$ around $x^\star$ so that $f(x) \geq f(x^\star)$ for all $x \in \mathcal{N}$.
- **global minimizer** if $f(x) \geq f(x^\star)$ for all $x \in \mathcal{D}$.
- **strict local minimizer** if there is a neighborhood $\mathcal{N}$ around $x^\star$ so that $f(x) > f(x^\star)$ 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 $x^\star \in \mathbf{R}^n$ *is a local minimizer of a differentiable function* $f : \mathbf{R}^n \to \mathbf{R}$, *then* $\nabla f(x^\star) = 0$.

First order optimality condition

Theorem

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

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

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

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

Second order optimality condition

Theorem

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

Second order optimality condition

Theorem

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

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

Outline

Linear program

a **linear program** is written as

$$\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & b - Ax \geq 0 \\ \text{variable} & x \in \mathbf{R}^n \end{array}$$

where

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- $b \in \mathbf{R}^m$: vector
- $c \in \mathbf{R}^n$: vector

how to solve?

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how to solve?

- use the simplex method
- use a conic solver

Conic form

conic form optimization problem generalizes LP:

$$\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & b - Ax \in \mathcal{K}, \end{array}$$

where $\mathcal{K}$ is a **convex cone**:

$$x \in \mathcal{K} \iff rx \in \mathcal{K} \text{ for any } r > 0.$$

examples:

- zero cone $\mathcal{K}_0 = \{0\}$
- positive orthant $\mathcal{K}_+ = \{x : x_i >= 0, \; i = 1, \ldots, n\}$
- second order cone $\mathcal{K}_{\mathrm{SOC}} = \{(x, t) : \|x\|_2 \leq t\}$
- positive semidefinite (PSD) cone $\mathcal{K}_{\mathrm{SDP}} = \{X : X = X^T, \; v^T X v \geq 0, \; \forall v \in \mathbf{R}^n\}$
- cartesian products of cones

Conic form: how to solve?

Morally, conic problems are solved by reducing to a nonlinear optimization problem

- barrier methods (*e.g.*, interior point methods)
  - add a barrier term to the objective that goes to infinity when constraints are violated
- penalty methods (*e.g.*, augmented Lagrangian methods, ADMM, ...)
  - add a penalty term to the objective that depends on a dual variable
  - adjust the dual variable to enforce constraints

Conic form example: nonnegative least squares

$$\begin{array}{ll} \text{minimize} & \|Ax - b\| \\ \text{subject to} & x \geq 0 \end{array}$$

$$\Updownarrow$$

$$\begin{array}{ll} \text{minimize} & t \\ \text{subject to} & x \in \mathcal{K}_+ \\ & (Ax - b, t) \in \mathcal{K}_{\text{SOC}} \end{array}$$

Conic form example: SVM

$$\begin{array}{ll}
\text{minimize} & \sum_{i=1}^{m} \max(0, 1 - b_i a_i^T x) + \|x\|^2 \\
\text{variable} & x \in \mathbf{R}^n
\end{array}$$

$$\Updownarrow$$

$$\begin{array}{ll}
\text{minimize} & \sum_i s_i + t \\
\text{subject to} & s \geq \mathbf{diag}(b) A x - 1 \\
& s \geq 0 \\
& t \geq \|x\|^2
\end{array}$$

$$\Updownarrow$$

$$\begin{array}{ll}
\text{minimize} & \sum_i s_i + t \\
\text{subject to} & s - \mathbf{diag}(b) A x + 1 \in \mathcal{K}_+ \\
& s \in \mathcal{K}_+ \\
& [t \;\, x; x^T \;\, I_n] \in \mathcal{K}_{\mathrm{SDP}}
\end{array}$$

Schur complement

Consider the block matrix

$$X = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}.$$

- the **Schur complement** of A in X is $C - B^T A^{-1} B$.
- $X \succeq 0$ if and only if $A \succeq 0$ and $C - B^T A^{-1} B \succeq 0$.
  (proof by partial minimization of quadratic form $(u, v)^T X (u, v)$ over $u \in \mathbf{R}^m$ for fixed $v \in \mathbf{R}^n$)

Conic form example: semidefinite programming

$$\begin{array}{ll} \text{minimize} & \lambda_{\max}(X) + y^T X^{-1} y \\ \text{subject to} & X \succeq 0 \end{array}$$

$$\Updownarrow$$

Conic form example: semidefinite programming

$$
\begin{array}{ll}
\text{minimize} & \lambda_{\max}(X) + y^T X^{-1} y \\
\text{subject to} & X \succeq 0
\end{array}
$$

$$\Updownarrow$$

$$
\begin{array}{ll}
\text{minimize} & t_1 + t_2 \\
\text{subject to} & t_1 I - X \in \mathcal{K}_{\mathrm{SDP}} \\
& \begin{bmatrix} t_2 & y^T \\ y & X \end{bmatrix} \in \mathcal{K}_{\mathrm{SDP}}
\end{array}
$$

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integer linear programming generalizes linear programming:

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variants:

- **mixed integer linear programming** (MILP): $x \in \mathbf{Z}^{n-m} \cup \mathbf{R}^m$
- **mixed integer nonlinear programming** (MINLP): $x \in \mathbf{Z}^{n-m} \cup \mathbf{R}^m$ and nonlinear objective or constraints

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how to solve?

- use Gurobi, CPLEX, ...
- branch and bound and cut (*i.e.*, a sequence of LPs)
- use duality to decompose into a sequence of simpler LPs

Outline

Quadratic optimization

Nonlinear optimization

Conic optimization

Integer programming

Convex optimization

Convex sets

Definition

A set $S \subseteq \mathbf{R}^n$ 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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quadratic, l1, 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

duality, stopping conditions, . . .

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- a function f is concave if $-f$ is convex
- concave maximization results in a **convex** optimization problem

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Theorem

If $x^\star$ is a local minimizer of a convex function f, then $x^\star$ is a global minimizer.

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

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Q: Is a global minimizer of a convex function always unique?
A: No. Picture.

Modern solvers

- algebraic modeling languages, *e.g.*
  - JuMP facilitates nonlinear and mixed integer optimization
  - CVX* (CVX, CVXPY, Convex.jl, ...) transform a problem into conic form
- and modern solvers

Optimization modeling

- Rocket control
- Power systems
- AML

Announcements

- website: https://stanford-cme-307.github.io/web
- Ed for discussion and announcements: https://edstem.org/us/courses/51411/
- fill out course survey (also linked on website): https://forms.gle/7hPniFeC576S12FAA
- talk to me after class and/or schedule office hours (see website)
- class attendance is required. will post some slides, generally no recordings