CME 307 / MS&E 311 / OIT 676: Optimization

Gradient descent

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October 24, 2025

Outline

Unconstrained minimization

Quadratic approximations

Analysis via Polyak-Lojasiewicz condition

Unconstrained minimization

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

- $f : \mathbb{R}^n \to \mathbb{R}$ differentiable
- assume optimal value $f^\star = \inf_x f(x)$ is attained (and finite)
- assume a starting point $x^{(0)}$ is known

unconstrained minimization methods

- produce sequence of points $x^{(k)}$, $k = 0, 1, \dots$ with

$$f(x^{(k)}) \to f^\star$$

(we hope)

Gradient descent

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

idea: go downhill

Algorithm Gradient descent

Given: $f : \mathbb{R}^d \to \mathbb{R}$, stepsize t, maxiters
Initialize: $x = 0$ (or anything you'd like)
For: $k = 1, \ldots,$ maxiters

▶ update x:

$$x \leftarrow x - t\nabla f(x)$$

Gradient descent: choosing a step-size

▶ **constant step-size.** $t^{(k)} = t$ (constant)
▶ **decreasing step-size.** $t^{(k)} = 1/k$
▶ **line search.** try different possibilities for $t^{(k)}$ until objective at new iterate

$$f(x^{(k)}) = f(x^{(k-1)} - t^{(k)} \nabla f(x^{(k-1)}))$$

decreases enough.

tradeoff: line search requires evaluating $f(x)$ (can be expensive)

Line search

define $x^+ = x - t\nabla f(x)$

- exact line search: find t to minimize $f(x^+)$
- the **Armijo rule** requires t to satisfy

$$f(x^+) \leq f(x) - ct\|\nabla f(x)\|^2$$

for some $c \in (0,1)$, e.g., $c = .01$.

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a simple **backtracking line search** algorithm:

- ▶ set $t = 1$
- ▶ if step decreases objective value sufficiently, accept x^+:

$$f(x^+) \leq f(x) - ct\|\nabla f(x)\|^2 \quad \implies \quad x \leftarrow x^+$$

  otherwise, halve the stepsize $t \leftarrow t/2$ and try again

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Q: can we can always satisfy the Armijo rule for some t?
A: yes! see gradient descent demo

Demo: gradient descent

https://github.com/stanford-cme-307/demos/blob/main/gradient-descent.ipynb

How well does GD work?

for $x \in \mathbb{R}^n$,

- $f(x) = x^T x$
- $f(x) = x^T A x$ for $A \succeq 0$
- $f(x) = \|x\|_1$ (nonsmooth but differentiable **almost** everywhere)
- $f(x) = 1/x$ on $x > 0$ (strictly convex but not strongly convex)

https:
//github.com/stanford-cme-307/demos/blob/main/gradient-descent-contours.ipynb

Outline

Quadratic approximation

Suppose $f : \mathbb{R} \to \mathbb{R}$ is twice differentiable. For any $x \in \mathbb{R}$, approximate f about x:

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

If f is a quadratic function, $\nabla^2 f(x) = H$ is constant.

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Quadratic approximations are useful because quadratics are easy to minimize:

$$
\begin{aligned}
y^\star &= \operatorname*{argmin}_{y} f(x) + \nabla f(x)^T (y - x) + \frac{1}{2}(y - x)^T H(y - x) \\
&\implies \nabla f(x) + H(y^\star - x) = 0 \\
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\end{aligned}
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If we approximate the Hessian of f by $H = \frac{1}{t}I$ for some $t > 0$ and choose x^+ to minimize the quadratic approximation, we obtain the **gradient descent** update with step size t:

$$x^+ = x + -t\nabla f(x)$$

Quadratic upper bound

Definition (Smooth)

A function $f : \mathbb{R} \to \mathbb{R}$ is *L*-**smooth** if for all $x, y \in \mathbb{R}$,

$$f(y) \leq f(x) + \nabla f(x)^T (y - x) + \frac{L}{2} \|y - x\|^2.$$

Equivalently, assuming the derivatives exist,

▶ the operator ∇f is *L*-**Lipschitz continuous**:

$$\|\nabla f(y) - \nabla f(x)\| \leq L\|y - x\|$$

▶ $\nabla^2 f(x) \preceq LI$ for all $x \in \mathbf{dom}\, f$.

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A: $\lambda_{\max}(A)$-smooth

Quadratic lower bound

Definition (Strongly convex)

A function $f : \mathbb{R} \to \mathbb{R}$ is μ-**strongly convex** for $\mu > 0$ if for all $x, y \in \mathbb{R}$,

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{\mu}{2} \|y - x\|^2.$$

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A: $\lambda_{\min}(A)$-strongly convex

Some important functions

for $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $x \in \mathbb{R}^n$,

- **Quadratic loss.** $\|Ax - b\|^2$
- **Logistic loss.** $f(x) = \sum_{i=1}^{m} \log(1 + \exp(b_i a_i^T x))$
  where a_i is ith row of A

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Q: Which of these are smooth? Under what conditions?
A: Both.
Q: Which of these are strongly convex? Under what conditions?
A: Quadratic loss is strongly convex if A is rank n. Logistic loss is strongly convex on a compact domain if A is rank n.

Optimizing the upper bound

start at $x^{(0)}$. suppose f is L-smooth, so for all $y \in \mathbb{R}$,

$$f(y) \leq f(x^{(0)}) + \nabla f(x)^T (y - x^{(0)}) + \frac{L}{2} \|y - x^{(0)}\|^2$$

let's choose next iterate $x^{(1)}$ to minimize this upper bound:

$$
\begin{aligned}
x^{(1)} &= \operatorname*{argmin}_y f(x) + \nabla f(x)^T (y - x) + \frac{L}{2} \|y - x\|^2 \\
&\implies \nabla f(x^{(0)}) + L(x^{(1)} - x^{(0)}) = 0 \\
x^{(1)} &= x^{(0)} - \frac{1}{L} \nabla f(x^{(0)})
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Optimizing the upper bound

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▶ **gradient descent** update with step size $t = \frac{1}{L}$
▶ lower bound ensures true optimum can't be too far away, and can be used to prove convergence

Outline

The Polyak-Lojasiewicz condition

Definition (Polyak-Lojasiewicz condition)

A function $f : \mathbb{R} \to \mathbb{R}$ satisfies the **Polyak-Lojasiewicz condition** if

$$\frac{1}{2}\|\nabla f(x)\|^2 \geq \mu(f(x) - f^\star)$$

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Theorem ([Karimi, Nutini, and Schmidt (2016)])

Suppose $f(x) = g(Ax)$ where $g : \mathbb{R}^m \to \mathbb{R}$ is strongly convex and $A : \mathbb{R}^n \to \mathbb{R}^m$ is linear. Then f is Polyak-Lojasiewicz.

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Q: Are all Polyak-Lojasiewicz functions convex?

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so logistic loss (on a compact set) and quadratic loss are Polyak-Lojasiewicz even when $m < n$

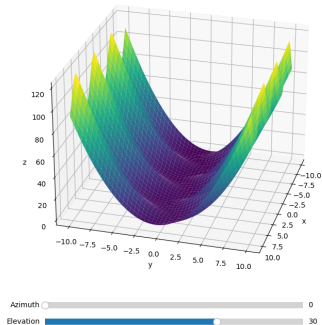**Q:** Are all Polyak-Lojasiewicz functions convex?

A: No. A river valley is Polyak-Lojasiewicz but not convex.

why use Polyak-Lojasiewicz? Polyak-Lojasiewicz is weaker than strong convexity and yields simpler proofs

River valley

$$f(x, y) = (y - \sin(x))^2$$

3D Plot of (Y - np.sin(X))**2 + .2*X

Azimuth ⎯○⎯⎯⎯⎯⎯⎯⎯⎯⎯⎯⎯⎯ 0
Elevation ⎯⎯⎯⎯⎯⎯○⎯⎯⎯⎯⎯⎯⎯ 30

PL and invexity

Theorem

Every Polyak-Lojasiewicz function is invex. (That is, any stationary point of a Polyak-Lojasiewicz function is globally optimal.)

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Theorem

Every Polyak-Lojasiewicz function is invex. (That is, any stationary point of a Polyak-Lojasiewicz function is globally optimal.)

proof: if $\nabla f(\bar{x}) = 0$, then

$$0 = \frac{1}{2}\|\nabla f(x)\|^2 \geq \mu(f(\bar{x}) - f^\star) \geq 0$$

$\implies f(\bar{x}) = f^\star$ is the global optimum.

strong convexity $\implies$ Polyak-Lojasiewicz

Theorem

If f is μ-strongly convex, then f is μ-Polyak-Lojasiewicz.

strong convexity $\implies$ Polyak-Lojasiewicz

Theorem

If f is μ-strongly convex, then f is μ-Polyak-Lojasiewicz.

proof: minimize the strong convexity condition over y:

$$\begin{aligned}
\min_y f(y) &\geq \min_y \left(f(x) + \nabla f(x)^T (y - x) + \frac{\mu}{2} \|y - x\|^2 \right) \\
f^\star &\geq f(x) - \frac{1}{2\mu} \|\nabla f(x)\|^2
\end{aligned}$$

since $y = x - \nabla f(x)/\mu$ minimizes the strong convexity upper bound

Types of convergence

▶ objective converges

$$f(x^{(k)}) \to f^\star$$

▶ iterates converge

$$x^{(k)} \to x^\star$$

under

▶ strong convexity: objective converges $\implies$ iterates converge
  proof: use strong convexity with $x = x^\star$ and $y = x^{(k)}$:

$$f(x^{(k)}) - f^\star \geq \frac{\mu}{2}\|x^{(k)} - x^\star\|^2$$

▶ Polyak-Lojasiewicz: not necessarily true ($x^\star$ may not be unique)

Rates of convergence

▶ linear convergence with rate c

$$f(x^{(k)}) - f^\star \leq c^k(f(x^{(0)}) - f^\star)$$

   ▶ looks like a line on a semi-log plot
   ▶ example: gradient descent on smooth strongly convex function
▶ sublinear convergence
   ▶ looks slower than a line (curves up) on a semi-log plot
   ▶ example: $1/k$ convergence

$$f(x^{(k)}) - f^\star \leq \mathcal{O}(1/k)$$

   ▶ example: gradient descent on smooth convex function
   ▶ example: stochastic gradient descent

Gradient descent converges linearly

Theorem

If $f : \mathbb{R}^n \to \mathbb{R}$ is μ-Polyak-Lojasiewicz, L-smooth, and $x^\star = \mathrm{argmin}_x f(x)$ exists, then gradient descent with stepsize L

$$x^{(k+1)} = x^{(k)} - \frac{1}{L}\nabla f(x^{(k)})$$

converges linearly to $f^\star$ with rate $(1 - \frac{\mu}{L})$.

Gradient descent converges linearly: proof

proof: plug in update rule to L-smoothness condition

$$
\begin{aligned}
f(x^{(k+1)}) - f(x^{(k)}) &\leq \nabla f(x^{(k)})^T (x^{(k+1)} - x^{(k)}) + \frac{L}{2}\|x^{(k+1)} - x^{(k)}\|^2 \\
&\leq (-\frac{1}{L} + \frac{1}{2L})\|\nabla f(x^{(k)})\|^2 \\
&\leq -\frac{1}{2L}\|\nabla f(x^{(k)})\|^2 \\
&\leq -\frac{\mu}{L}(f(x^{(k)}) - f^\star) \qquad \triangleright \text{(using PL)}
\end{aligned}
$$

Gradient descent converges linearly: proof

proof: plug in update rule to L-smoothness condition

$$
\begin{aligned}
f(x^{(k+1)}) - f(x^{(k)}) &\leq \nabla f(x^{(k)})^T (x^{(k+1)} - x^{(k)}) + \frac{L}{2} \|x^{(k+1)} - x^{(k)}\|^2 \\
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&\leq -\frac{\mu}{L} (f(x^{(k)}) - f^\star) \qquad \triangleright \text{(using PL)}
\end{aligned}
$$

decrement proportional to error $\implies$ linear convergence:

$$
\begin{aligned}
f(x^{(k)}) - f^\star &\leq (1 - \frac{\mu}{L})(f(x^{(k-1)}) - f^\star) \\
&\leq \left(1 - \frac{\mu}{L}\right)^k (f(x^{(0)}) - f^\star)
\end{aligned}
$$

Practical convergence

▶ Gradient descent with optimal stepsize converges even faster.

$$f(x^{(k+1)}) = \inf_{\alpha} f(x^{(k)} - \alpha \nabla f(x^{(k)})) \leq f(x^{(k)} - \frac{1}{L} \nabla f(x^{(k)}))$$

Practical convergence

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▶ Local vs global convergence

Outline

Applications of quadratic programs

Classification

Quadratic program: application

Markowitz portfolio optimization problem:

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

where

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

Quadratic program: application

control system design problem:

$$x^+ = Ax + Bu$$

- $x \in \mathbb{R}^n$: state (e.g., position, velocity)
- $u \in \mathbb{R}^m$: control (e.g., force, torque)

$$\begin{array}{ll} \text{minimize} & \sum_{t=1}^{T} x_t^T Q x_t + u_t^T R u_t \\ \text{subject to} & x_{t+1} = A x_t + B u_t, \quad t = 0, \ldots, T-1 \\ & x_0 = x^{\text{init}} \end{array}$$

Outline

Application: classification

classification problem: m data points

- feature vector $a_i \in \mathbb{R}^n$, $i = 1, \ldots, m$
- 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**

$$\text{minimize} \quad \sum_{i=1}^{m} \log(1 + \exp\left(-b_i a_i^T x\right)) + r(x)$$
$$\text{variable} \quad x \in \mathbb{R}^n$$

where

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

Support vector machine

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

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

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

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where $b_i \in \{-1, 1\}$ and $a_i \in \mathbb{R}^n$. not differentiable!

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