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

Gradient descent

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Outline

Unconstrained minimization

Quadratic approximations

Analysis via Polyak-Lojasiewicz condition

Unconstrained minimization

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

- $f : \mathbf{R}^n \to \mathbf{R}$ 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 $x^{(k)}$, $k = 0, 1, \ldots$ with

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

(we hope)

Gradient descent

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

idea: go downhill

Algorithm Gradient descent

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

- 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^+:

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

  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 $x \in \mathbf{R}^n$,

- $f(x) = x^T x$
- $f(x) = x^T A x$ 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 $f : \mathbf{R} \to \mathbf{R}$ is twice differentiable. For any $x \in \mathbf{R}$, 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:

$$\begin{aligned} y^\star &= \operatorname*{argmin}_y f(x) + \nabla f(x)^T(y-x) + \frac{1}{2}(y-x)^T H(y-x) \\ &\implies \nabla f(x) + H(y^\star - x) = 0 \\ y^\star &= x - H^{-1}(\nabla f(x)). \end{aligned}$$

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

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

Equivalently, assuming the derivatives exist,

- the operator $\frac{1}{L}\nabla f$ 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

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Definition (Strongly convex)

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

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

Some important functions

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

- **Quadratic loss.** $\|Ax - b\|^2$
- **Logistic loss.** $f(x) = \sum_{i=1}^m \log(1 + \exp\left(b_i a_i^T x\right))$
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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 $y \in \mathbf{R}$,

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

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

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

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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

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Analysis via Polyak-Lojasiewicz condition

The Polyak-Lojasiewicz condition

Definition (Polyak-Lojasiewicz condition)

A function $f : \mathbf{R} \to \mathbf{R}$ 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* $g : \mathbf{R}^m \to \mathbf{R}$ *is strongly convex and* $A : \mathbf{R}^n \to \mathbf{R}^m$ *is linear. Then* f *is Polyak-Lojasiewicz.*

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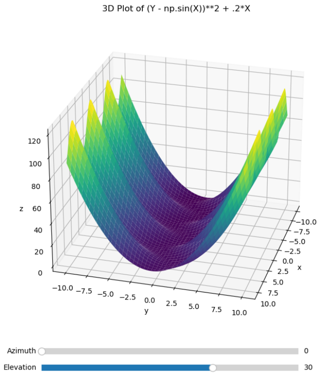
Q: Are all Polyak-Lojasiewicz functions convex?
A: No. A river valley is Polyak-Lojasiewicz but not convex.
why use Polyak-Lojasiewicz? Polyak-Lojasiewicz is weaker than strong convexity and yields simpler proofs

River valley

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



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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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.

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Theorem

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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 $f : \mathbf{R}^n \to \mathbf{R}$ 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

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

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\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.

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

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- Local vs global convergence

Quiz

- A strongly convex function always satisfies the Polyak-Lojasiewicz condition
  A. true
  B. false
- Suppose $f : \mathbf{R} \to \mathbf{R}$ is L-smooth and satisfies the Polyak-Lojasiewicz condition. Then any stationary point $\nabla f(x) = 0$ of f is a global optimum: $f(x) = \mathrm{argmin}_y f(y) =: f^\star$.
  A. true
  B. false
- Suppose $f : \mathbf{R} \to \mathbf{R}$ is L-smooth and satisfies the Polyak-Lojasiewicz condition. Then gradient descent on f converges linearly from any starting point.
  A. true
  B. false

Outline

Applications of quadratic programs

Classification

Quadratic program: application

Markowitz portfolio optimization problem:

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

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

Quadratic program: application

control system design problem:

$$x^+ = Ax + Bu$$

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

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

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Applications of quadratic programs

Classification

Application: 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 $b_i a^T x > 0$

Application: classification

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

- 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