

# 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

minimize  $f(x)$

- ▶  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  differentiable
- ▶ assume optimal value  $f^* = \inf_x f(x)$  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

$$f(x^{(k)}) \rightarrow f^*$$

(we hope)

## Gradient descent

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

idea: go downhill

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**Algorithm** Gradient descent

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**Given:**  $f : \mathbb{R}^d \rightarrow \mathbb{R}$ , stepsize  $t$ , maxiters

**Initialize:**  $x = 0$  (or anything you'd like)

**For:**  $k = 1, \dots, \text{maxiters}$

- ▶ update  $x$ :

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

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## 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  $x^+$ :

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

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

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**Q:** can we 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  $x \in \mathbb{R}^n$ ,

- ▶  $f(x) = x^T x$
- ▶  $f(x) = x^T Ax$  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)

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Unconstrained minimization

Quadratic approximations

Analysis via Polyak-Lojasiewicz condition

## Quadratic approximation

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

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

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Quadratic approximations are useful because quadratics are easy to minimize:

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

$$y^* = x - H^{-1}(\nabla f(x)).$$

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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  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is  **$L$ -smooth** if for all  $x, y \in \mathbb{R}^n$ ,

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Equivalently, assuming the derivatives exist,

- ▶ the operator  $\nabla f$  is  **$L$ -Lipschitz continuous**:

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

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

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

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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  $i$ th row of  $A$

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**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:

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

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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

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## The Polyak-Lojasiewicz condition

Definition (Polyak-Lojasiewicz condition)

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

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

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

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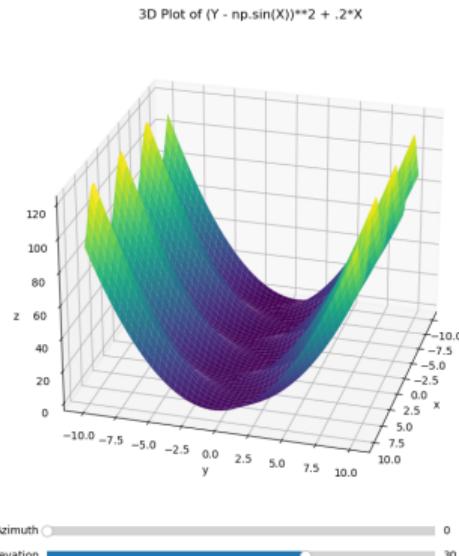
**Q:** Are all Polyak-Lojasiewicz functions convex?

**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

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



## Optimality condition for PL function

### Theorem

*Any stationary point of a Polyak-Lojasiewicz function is globally optimal.*

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

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

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

**strong convexity  $\implies$  Polyak-Lojasiewicz**

### Theorem

*If  $f$  is  $\mu$ -strongly convex, then  $f$  is  $\mu$ -Polyak-Lojasiewicz.*

## strong convexity $\implies$ Polyak-Lojasiewicz

### Theorem

If  $f$  is  $\mu$ -strongly convex, then  $f$  is  $\mu$ -Polyak-Lojasiewicz.

**proof:** minimize the strong convexity condition over  $y$ :

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

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

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

## Types of convergence

- ▶ objective converges

$$f(x^{(k)}) \rightarrow f^*$$

- ▶ iterates converge

$$x^{(k)} \rightarrow x^*$$

under

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

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

- ▶ Polyak-Łojasiewicz: not necessarily true ( $x^*$  may not be unique)

## Rates of convergence

- ▶ linear convergence with rate  $c$

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

- ▶ 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

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

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

## Gradient descent converges linearly

### Theorem

If  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is  $\mu$ -Polyak-Lojasiewicz,  $L$ -smooth, and  $x^* = \operatorname{argmin}_x f(x)$  exists, then gradient descent with stepsize  $L$

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

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

## Gradient descent converges linearly: proof

**proof:** plug in update rule to  $L$ -smoothness condition

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

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decrement proportional to error  $\implies$  linear convergence:

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

## 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

# 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)

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

# Outline

Applications of quadratic programs

Classification

## Application: classification

**classification** problem:  $m$  data points

- ▶ feature vector  $a_i \in \mathbb{R}^n$ ,  $i = 1, \dots, m$
- ▶ label  $b_i \in \{-1, 1\}$ ,  $i = 1, \dots, m$

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**

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

where

- ▶  $b_i \in \{-1, 1\}$ ,  $a_i \in \mathbb{R}^n$
- ▶  $r : \mathbb{R}^n \rightarrow \mathbb{R}$  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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how to solve?

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