COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2023.

Lecture 23

Logistics

- Problem Set 5 is posted. It can be turned in up to 12/11 (next Monday) at 11:59pm It is optional – the core problems can replace the lowest of your previous four core problem grades.
- The final will be on 12/14 in this room, 10:30am-12:30pm.
- See Piazza for additional final review office ours schedule.
- See website/Moodle for final prep material.

Summary

Last Class:

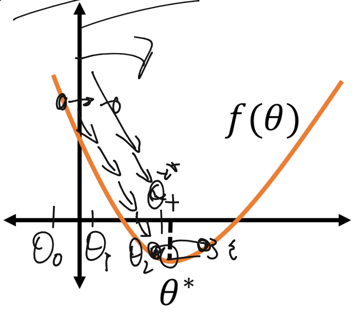
- Multivariable calculus review and gradient computation.
- Introduction to gradient descent. Motivation as a greedy algorithm.
- Convex functions

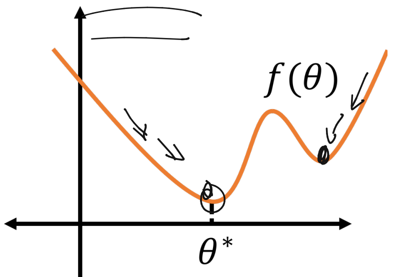
This Class:

- Analysis of gradient descent for Lipschitz, convex functions.
- Extension to projected gradient descent for constrained optimization.

When Does Gradient Descent Work?

$\theta \in \mathbb{R} \quad \nabla f(\theta) \in \mathbb{R}$





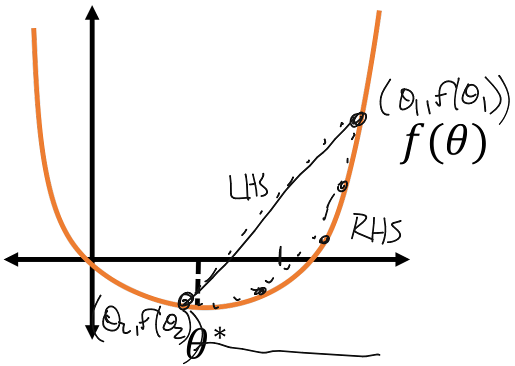
Gradient Descent Update: $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$

Definition – Convex Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$ and $\lambda \in [0, 1]$:

$$(1 - \lambda) \cdot f(\vec{\theta}_1) + \lambda \cdot f(\vec{\theta}_2) \geq f\left((1 - \lambda) \cdot \vec{\theta}_1 + \lambda \cdot \vec{\theta}_2\right)$$

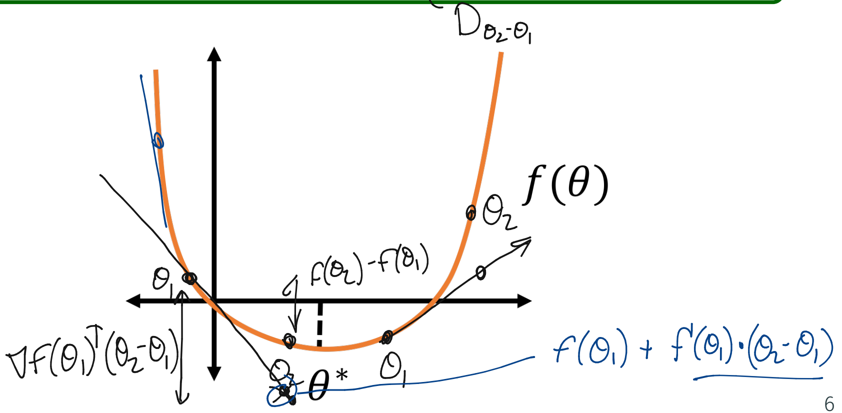
x^2

CX



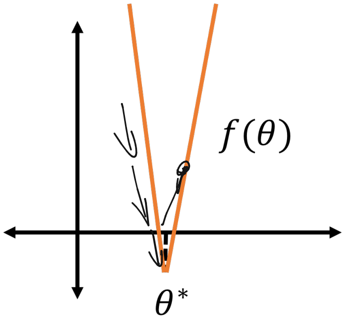
Corollary – Convex Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$ and $\lambda \in [0,1]$:

$$f(\vec{\theta}_2) - f(\vec{\theta}_1) \geq \vec{\nabla} f(\vec{\theta}_1)^T \left(\vec{\theta}_2 - \vec{\theta}_1\right)$$



Lipschitz Functions

$\theta \in \mathbb{R} \quad \nabla f(\theta) \in \mathbb{R}$



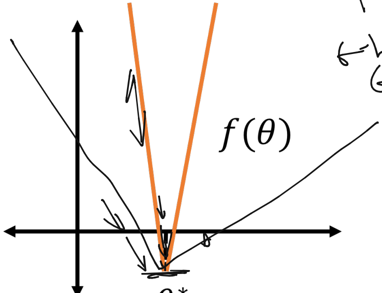
Gradient Descent Update:

$\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$

bigger step size
= larger error

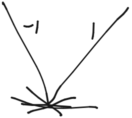
Lipschitz Functions

$\theta \in \mathbb{R} \quad \nabla f(\theta) \in \mathbb{R}$



$f(x) = |x|$

G-Lip for G = 1



relu

Gradient Descent Update:
$\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$

is $f(x) = x^2$ G-Lip..

for some G < ∞

$f'(x) = 2x$

Need to assume that the function is Lipschitz (size of gradient is bounded): There is some G s.t.:

$$\forall \vec{\theta} : \quad \|\vec{\nabla} f(\vec{\theta})\|_2 \leq G \Leftrightarrow \forall \vec{\theta}_1, \vec{\theta}_2 : \quad |f(\vec{\theta}_1) - f(\vec{\theta}_2)| \leq G \cdot \|\vec{\theta}_1 - \vec{\theta}_2\|_2$$

$|f'(\theta)| \leq G$

Well-Behaved Functions

Definition – Convex Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$ and $\lambda \in [0, 1]$:

$$(1-\lambda) \cdot f(\vec{\theta}_1) + \lambda \cdot f(\vec{\theta}_2) \geq f\left((1-\lambda) \cdot \vec{\theta}_1 + \lambda \cdot \vec{\theta}_2\right)$$

Corollary – Convex Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$ and $\lambda \in [0, 1]$:

$f(\theta_t) - f(\theta_i) \geq \nabla f(\theta_i)^T(\theta_t - \theta_i)$

$$f(\vec{\theta}_2) - f(\vec{\theta}_1) \geq \vec{\nabla} f(\vec{\theta}_1)^T \left(\vec{\theta}_2 - \vec{\theta}_1\right)$$

Definition – Lipschitz Function: A function $f : \mathbb{R}^d \to \mathbb{R}$ is G-Lipschitz if $\|\vec{\nabla} f(\vec{\theta})\|_2 \leq G$ for all $\vec{\theta}$.

GD Analysis – Convex Functions

Assume that:

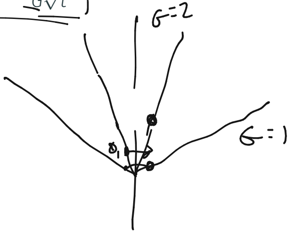
$\theta_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$ $\quad R = \|\theta_*\|$

- f is convex.
- f is G-Lipschitz.
- $\|\vec{\theta}_1 - \vec{\theta}_*\|_2 \leq R$ where $\vec{\theta}_1$ is the initialization point.

Gradient Descent

- Choose some initialization $\vec{\theta}_1$ and set $\eta = \frac{R}{G\sqrt{t}}$.
- For $i = 1, \ldots, t-1$
  - $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \vec{\nabla} f(\vec{\theta}_i)$
- Return $\hat{\theta} = \arg\min_{\vec{\theta}_1, \ldots, \vec{\theta}_t} f(\vec{\theta}_i)$.

θ_t



GD Analysis Proof

Theorem – GD on Convex Lipschitz Functions: For convex G-Lipschitz function f, GD run with $t \geq \frac{R^2G^2}{\epsilon^2}$ iterations, $\eta = \frac{R}{G\sqrt{t}}$, and starting point within radius R of $\vec{\theta}_*$, outputs $\hat{\theta}$ satisfying:

$$f(\hat{\theta}) \leq f(\vec{\theta}_*) + \epsilon.$$

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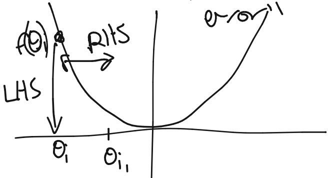
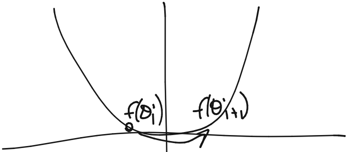
how much closer to θ* I move in step i

LHS — small

Step 1: For all i, $f(\vec{\theta}_i) - f(\vec{\theta}_*) \leq \frac{\|\vec{\theta}_i - \vec{\theta}_*\|_2^2 - \|\vec{\theta}_{i+1} - \vec{\theta}_*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$. Visually:

"function error"





Either f(θi) is small OR I move much closer to θ*.

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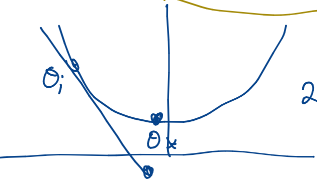
$$\|\theta_{i+1} - \theta_*\|_2^2 = \|\theta_i - \eta\nabla f(\theta_i) - \theta_*\|_2^2$$

$$= \|\theta_i - \theta_*\|_2^2 - 2\eta\nabla f(\theta_i)^T(\theta_i - \theta_*) + \|\eta\nabla f(\theta_i)\|_2^2$$

$\leq \eta^2 G^2$

$\geq f(\theta_i) - f(\theta_*)$



$$2\eta\nabla f(\theta_i)^T(\theta_i - \theta_*) \leq \|\theta_i - \theta_*\|_2^2 - \|\theta_{i+1} - \theta_*\|_2^2 + \eta^2 G^2$$

$$\nabla f(\theta_i)^T(\theta_i - \theta_*) \leq \frac{\|\theta_i - \theta_*\|_2^2 - \|\theta_{i+1} - \theta_*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$$

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$\nabla f(\theta_i)^T(\theta_i - \theta_*) \geq f(\theta_i) - f(\theta_*)$ by convexity

GD Analysis Proof

Theorem – GD on Convex Lipschitz Functions: For convex G-Lipschitz function f, GD run with $t \geq \frac{R^2 G^2}{\epsilon^2}$ iterations, $\eta = \frac{R}{G\sqrt{t}}$, and starting point within radius R of $\vec{\theta}_*$, outputs $\hat{\theta}$ satisfying:

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$\leq \epsilon$

Step 2: $\frac{1}{t}\sum_{i=1}^{t} f(\vec{\theta}_i) - f(\vec{\theta}_*) \leq \frac{R^2}{2\eta \cdot t} + \frac{\eta G^2}{2}$.

$$\frac{1}{2\eta t}\sum_{i=1}^{t} \|\theta_i - \theta_*\|_2^2 - \|\theta_{i+1} - \theta_*\|_2^2 + \frac{\eta G^2}{2} \leq \frac{R^2}{2\eta t} + \frac{\eta G^2}{2} \leq \epsilon$$

$$\|\theta_1 - \theta_*\|_2^2 - \|\theta_2 - \theta_*\|_2^2 + \|\theta_2 - \theta_*\| - \|\theta_3 - \theta_*\|_2^2 \cdots - \|\theta_{t+1} - \theta_*\|_2^2$$

$$\|\theta_1 - \theta_*\|_2^2 - \|\theta_{t+1} - \theta_*\|_2^2 \leq \|\theta_1 - \theta_*\|_2^2 \leq R^2$$

Theorem – GD on Convex Lipschitz Functions: For convex G-Lipschitz function f, GD run with $t \geq \frac{R^2G^2}{\epsilon^2}$ iterations, $\eta = \frac{R}{G\sqrt{t}}$, and starting point within radius R of $\vec{\theta}_*$, outputs $\hat{\theta}$ satisfying:

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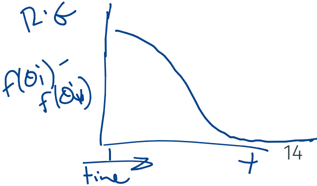
$\eta = \frac{R}{G\sqrt{t}}$, $t = \frac{R^2G^2}{\epsilon^2}$, $\sqrt{t} = \frac{RG}{\epsilon}$

$$\frac{R^2}{2\eta t} + \frac{\eta G^2}{2} = \frac{RG}{2\sqrt{t}} + \frac{RG}{2\sqrt{t}} = \frac{RG}{\sqrt{t}} = \frac{RG}{RG/\epsilon} = \epsilon$$

$$f(x) = (x-a)^2$$

$$f(\hat{\theta}) = \min_{i=1..t} f(\theta_i) \leq \frac{1}{t}\sum f(\theta_i)$$



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Constrained Convex Optimization

Often want to perform convex optimization with convex constraints.

$$\vec{\theta}^* = \arg\min_{\vec{\theta} \in \mathcal{S}} f(\vec{\theta}),$$

where $\mathcal{S}$ is a convex set.

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E.g. $\mathcal{S} = \{\vec{\theta} \in \mathbb{R}^d : \|\vec{\theta}\|_2 \leq 1\}$.

Projected Gradient Descent

For any convex set let $P_{\mathcal{S}}(\cdot)$ denote the projection function onto $\mathcal{S}$.

- $P_{\mathcal{S}}(\vec{y}) = \arg\min_{\vec{\theta} \in \mathcal{S}} \|\vec{\theta} - \vec{y}\|_2$.

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- For $\mathcal{S} = \{\vec{\theta} \in \mathbb{R}^d : \|\vec{\theta}\|_2 \leq 1\}$ what is $P_{\mathcal{S}}(\vec{y})$?
- For $\mathcal{S}$ being a k dimensional subspace of $\mathbb{R}^d$, what is $P_{\mathcal{S}}(\vec{y})$?

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Projected Gradient Descent

- Choose some initialization $\vec{\theta}_1$ and set $\eta = \frac{R}{G\sqrt{t}}$.
- For $i = 1, \ldots, t-1$
  - $\vec{\theta}_{i+1}^{(out)} = \vec{\theta}_i - \eta \cdot \vec{\nabla} f(\vec{\theta}_i)$
  - $\vec{\theta}_{i+1} = P_{\mathcal{S}}(\vec{\theta}_{i+1}^{(out)})$.
- Return $\hat{\theta} = \arg\min_{\vec{\theta}_i} f(\vec{\theta}_i)$.

Convex Projections

Projected gradient descent can be analyzed identically to gradient descent!

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Theorem – Projection to a convex set: For any convex set $\mathcal{S} \subseteq \mathbb{R}^d$, $\vec{y} \in \mathbb{R}^d$, and $\vec{\theta} \in \mathcal{S}$,

$$\|P_{\mathcal{S}}(\vec{y}) - \vec{\theta}\|_2 \leq \|\vec{y} - \vec{\theta}\|_2.$$

Projected Gradient Descent Analysis

Theorem – Projected GD: For convex G-Lipschitz function f, and convex set $\mathcal{S}$, Projected GD run with $t \geq \frac{R^2 G^2}{\epsilon^2}$ iterations, $\eta = \frac{R}{G\sqrt{t}}$, and starting point within radius R of $\vec{\theta}_*$, outputs $\hat{\theta}$ satisfying:

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Recall: $\vec{\theta}_{i+1}^{(out)} = \vec{\theta}_i - \eta \cdot \vec{\nabla} f(\vec{\theta}_i)$ and $\vec{\theta}_{i+1} = P_{\mathcal{S}}(\vec{\theta}_{i+1}^{(out)})$.

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Step 2: $\frac{1}{t}\sum_{i=1}^{t} f(\vec{\theta}_i) - f(\vec{\theta}_*) \leq \frac{R^2}{2\eta \cdot t} + \frac{\eta G^2}{2}$ $\implies$ Theorem.