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:

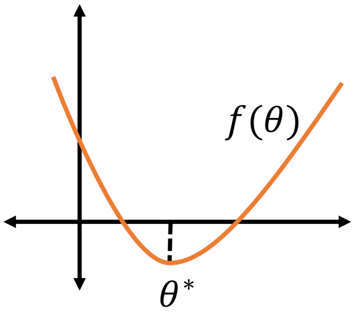
- Multivariable calculus review and gradient computation.
- Introduction to gradient descent. Motivation as a greedy algorithm.
- Convex functions

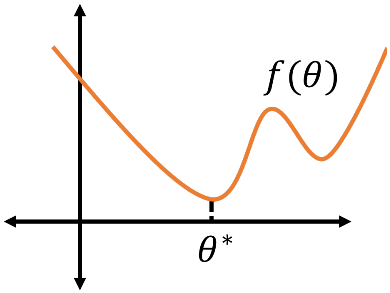
This Class:

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

When Does Gradient Descent Work?

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

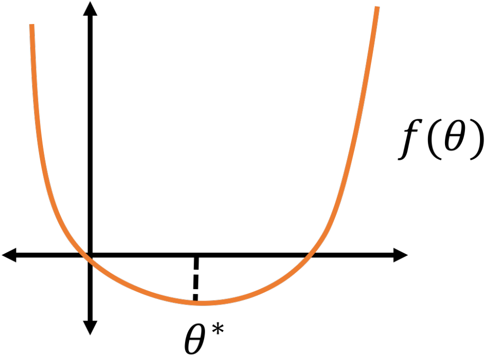




Gradient Descent Update: $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$

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 $\lambda \in [0, 1]$:

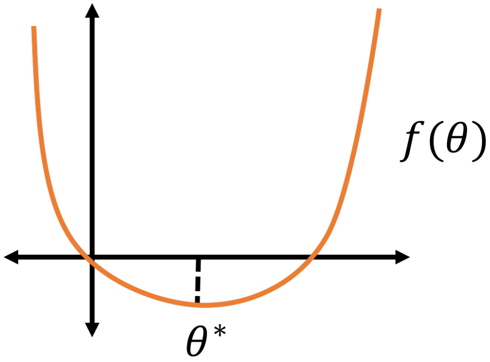
$$(1-\lambda)\cdot f(\vec{\theta}_1) + \lambda \cdot f(\vec{\theta}_2) \geq f\left((1-\lambda)\cdot \vec{\theta}_1 + \lambda \cdot \vec{\theta}_2\right)$$



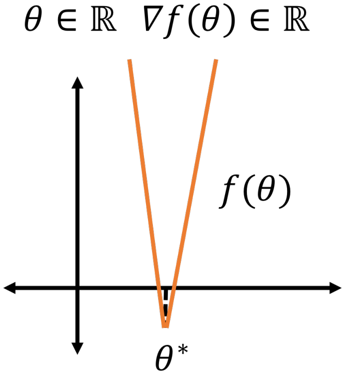
Convexity

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



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

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

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

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 $\lambda \in [0, 1]$:

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

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:

- 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 $\hat{\theta} = \arg\min_{\vec{\theta}_1, \ldots, \vec{\theta}_t} f(\vec{\theta}_i)$.

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:

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

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:

GD Analysis Proof

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

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

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

Step 1.1: $\vec{\nabla} f(\vec{\theta}_i)^T(\vec{\theta}_i - \vec{\theta}_*) \leq \frac{\|\vec{\theta}_i - \vec{\theta}_*\|_2^2 - \|\vec{\theta}_{i+1} - \vec{\theta}_*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$ $\implies$ Step 1 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:

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

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

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

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:

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

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

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:

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

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

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.

Definition – Convex Set: A set $\mathcal{S} \subseteq \mathbb{R}^d$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathcal{S}$ and $\lambda \in [0, 1]$:

$$(1 - \lambda)\vec{\theta}_1 + \lambda \cdot \vec{\theta}_2 \in \mathcal{S}$$

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 $\mathcal{S}$.

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

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!

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 $t \geq \frac{R^2G^2}{\epsilon^2}$ iterations, $\eta = \frac{R}{G\sqrt{t}}$, and starting point within radius R of $\vec{\theta}_*$, outputs $\hat{\theta}$ satisfying:

$$f(\hat{\theta}) \leq f(\vec{\theta}_*) + \epsilon = \min_{\vec{\theta} \in \mathcal{S}} f(\vec{\theta}) + \epsilon$$

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

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

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

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.