COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2024.

Lecture 23

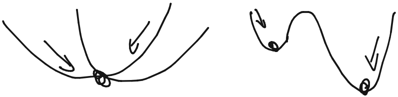
Logistics

- Problem Set 5 can be turned in up to 12/12 (next Thursday) at 11:59pm with no penalty. No extensions will be granted beyond this. The challenge problem is optional extra credit.
- After today you will be able to solve every problem on it.
- Additional final review office hours will be posted soon.

Summary

Last Class:

- Multivariable calculus review — gradient, directional derivative
- Introduction to gradient descent. Motivation as a greedy algorithm.



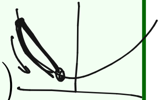
- Convex functions
- Lipschitz functions

This Class:

- Analysis of gradient descent for convex Lipschitz functions
- Extension to projected gradient descent for constrained optimization.
- Start on online/stochastic gradient descent?

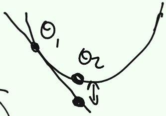
Well-Behaved Functions

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



$\theta_i = \theta_1$

$\theta_* = \theta_2$

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

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

$\nabla f(\theta_1)^T(\theta_1 - \theta_2) \geq f(\theta_1) - f(\theta_2)$

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 $\vec{\theta}$.

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.

G and R are known

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 θ_*, outputs $\hat{\theta}$ satisfying:

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

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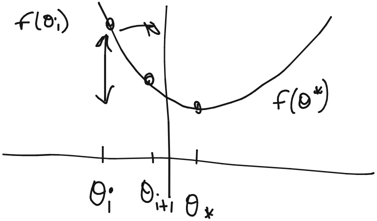
Step 1: For all i, $f(\vec{\theta}_i) - f(\vec{\theta}_*) \leq \frac{\|\vec{\theta}_i - \vec{\theta}_*\|_2^2 - \|\vec{\theta}_{i+1} - \vec{\theta}_*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$. Visually:

small



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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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$\theta_{i+1} = \theta_i - \eta \nabla f(\theta_i)$

divide by 2η

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

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

Step 1.1. $\Rightarrow$ Step 1

$\eta^2 \|\nabla f(\theta_i)\|_2^2 \leq \eta^2 G^2$

"progress towards opt"

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

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

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

GD Analysis Proof

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GD Analysis Proof

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

avg error $\leq \varepsilon \implies f(\hat{\theta}) - f(\theta^*) \leq \varepsilon$

"telescoping sum"

$$\frac{1}{t}\sum f(\theta_i) - f(\theta_*) \leq \frac{1}{t\,2\eta}\left[\sum_{i=1}^{t} \|\theta_i - \theta_*\|_2^2 - \|\theta_{i+1} - \theta_*\|_2^2\right] + \frac{\eta G^2}{2}$$ (by step 1)

how can I simplify?

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

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

$$\leq \boxed{\frac{R^2}{t\,2\eta} + \frac{\eta G^2}{2}}$$

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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$$\leq \frac{R^2}{\frac{2R}{G\sqrt{t}} \cdot t} + \frac{RG^2}{G\sqrt{t} \cdot 2} = \frac{RG}{2\sqrt{t}} + \frac{RG}{2\sqrt{t}} = \frac{RG}{\sqrt{t}}$$

$$t = \frac{R^2 G^2}{\varepsilon^2}$$

$$\leq \frac{RG}{\sqrt{\frac{R^2 G^2}{\varepsilon^2}}} = \varepsilon$$

GD Analysis Proof

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Constrained Convex Optimization

Often want to perform convex optimization with convex constraints.

$\theta^* = \arg\min f(\theta)$

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

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

Constrained Convex Optimization

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

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

Constrained Convex Optimization

Often want to perform convex optimization with convex constraints.

W1

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

$S : \{\theta \in \mathbb{R}^d : \theta = \underset{d \times k}{V} \underset{k \times 1}{c} \text{ for some } c\}$

is this convex?

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

$\theta_1, \theta_2 \in S$, $\underbrace{\lambda\theta_1 + (1-\lambda)\theta_2}_{\in S} = \lambda V c_1 + (1-\lambda) V c_2$
$= Vc \quad c = \lambda c_1 + (1-\lambda) c_2$

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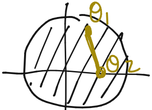
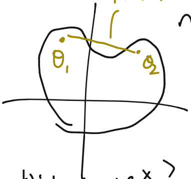
E.g. $\mathcal{S} = \{\vec{\theta} \in \mathbb{R}^d : \|\vec{\theta}\|_2 \leq 1\}$.

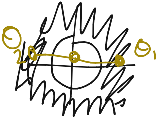


$\lambda\theta_1 + (1-\lambda)\theta_2 \notin S$

not convex



$S = \{\theta \in \mathbb{R}^d : \|\theta\|_2 \geq 1\}$ – is this convex?



Projected Gradient Descent

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

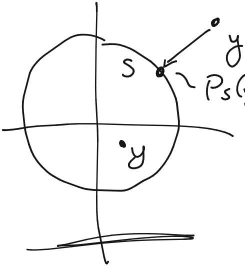
- $P_{\mathcal{S}}(\vec{y}) = \arg\min_{\vec{\theta} \in \mathcal{S}} \|\vec{\theta} - \vec{y}\|_2$.

("projection of y onto S"

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 $P_{\mathcal{S}}(\vec{y})$?



$$P_s(y) = \frac{y}{\|y\|} \quad \text{if } \|y\| \geq 1$$
$$= y \quad \text{if } \|y\| \leq 1$$

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

$P_S(y) = VV^T y$ where V is orthonormal basis for S.

Projected Gradient Descent

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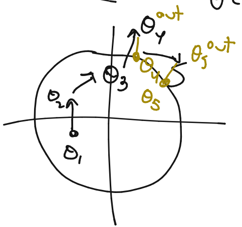
Projected Gradient Descent

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

$\underset{\theta \in S}{\arg\min} \; f(\theta)$



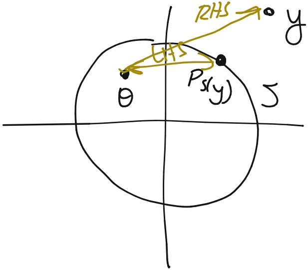
Convex Projections

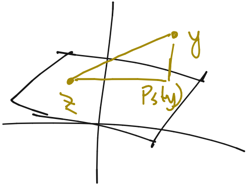
Projected gradient descent can be analyzed identically to gradient descent!

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 $\vec{\theta} \in \mathcal{S}$,

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





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:

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

Projected Gradient Descent Analysis

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

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θ_{i+1}^{out}

(follows from GD analysis)

$\|\theta_{i+1}^{out} - \theta_*\|_2^2 \geq \|\theta_{i+1} - \theta_*\|_2^2$ (by convexity of S)

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exactly what we had for GD

Projected Gradient Descent Analysis

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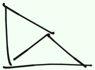

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Step 2: $\frac{1}{t} \sum_{i=1}^{t} f(\vec{\theta}_i) - f(\vec{\theta}_*) \leq \frac{R^2}{2\eta \cdot t} + \frac{\eta G^2}{2}$ $\Longrightarrow$ Theorem.

Typical Optimization Problem in Machine Learning: Given data points $\vec{x}_1, \ldots, \vec{x}_n$ and labels/observations $y_1, \ldots, y_n$ solve:

$$\vec{\theta}^* = \underset{\vec{\theta} \in \mathbb{R}^d}{\arg\min}\, L(\vec{\theta}, \mathbf{X}, y) = \sum_{j=1}^{n} \ell(M_{\vec{\theta}}(\vec{x}_j), y_j).$$

prediction error for training point j

Gradient Descent At Scale

Typical Optimization Problem in Machine Learning: Given data points $\vec{x}_1, \ldots, \vec{x}_n$ and labels/observations $y_1, \ldots, y_n$ solve:

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The gradient of $L(\vec{\theta}, \mathrm{X})$ has one component per data point:

$$\vec{\nabla} L(\vec{\theta}, \mathrm{X}, y) = \sum_{j=1}^{n} \vec{\nabla} \ell(M_{\vec{\theta}}(\vec{x}_j), y_j).$$

Gradient Descent At Scale

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The gradient of $L(\vec{\theta}, \mathbf{X})$ has one component per data point:

$$\vec{\nabla} L(\vec{\theta}, \mathbf{X}) = \sum_{j=1}^{n} \vec{\nabla} \ell(M_{\vec{\theta}}(\vec{x}_j), y_j).$$

When n is large this is very expensive to compute! $O(n)$

Gradient Descent At Scale

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- The key idea behind **stochastic gradient descent** (SGD).

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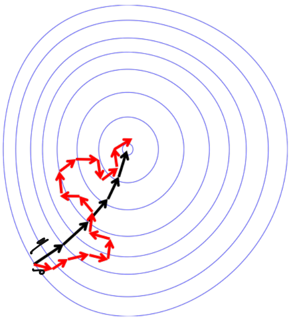

$$\vec{\theta}^{(i+1)} = \vec{\theta}^{(i)} - \eta \cdot \vec{\nabla} L(\vec{\theta}^{(i)}, X) \text{ vs. } \vec{\theta}^{(i+1)} = \vec{\theta}^{(i)} - \eta \cdot \vec{\nabla} \ell(M_{\vec{\theta}^{(i)}}(\vec{x}_j), y_j)$$

Online Gradient Descent

SGD is closely related to online gradient descent.