COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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Lecture 23

Last Class:

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

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

This Class:

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

Goal: Find $\vec{\theta} \in \mathbb{R}^d$ that (nearly) minimizes convex function f.

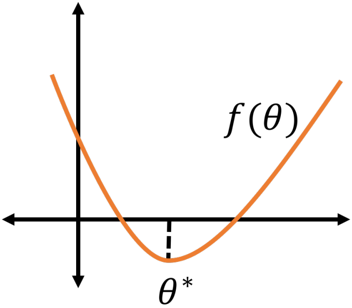
Gradient Descent Algorithm:

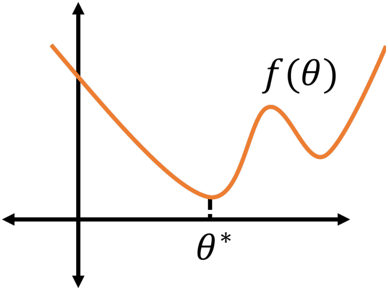
- Choose some initialization $\vec{\theta}^{(0)}$.
- For $i = 1, \ldots, t-1$
  - $\vec{\theta}^{(i)} = \vec{\theta}^{(i-1)} - \eta \nabla f(\vec{\theta}^{(i-1)})$
- Return $\hat{\theta} = \arg\min_{\vec{\theta}_1, \ldots \vec{\theta}_t} f(\vec{\theta}_i)$.

Step size η is chosen ahead of time or adapted during the algorithm. For now assume η stays the same in each iteration.

WHEN DOES GRADIENT DESCENT WORK?

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

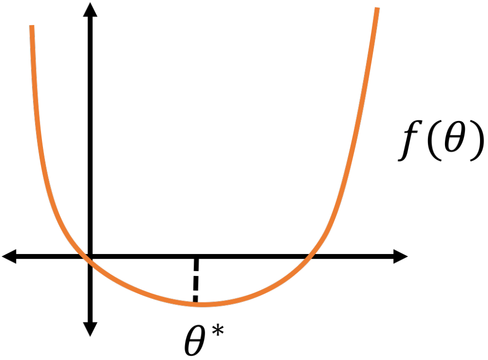




Gradient Descent Update in 1D: $\theta_{i+1} = \theta_i - \eta f'(\theta_i)$, i.e., increase θ if derivative is negative and decrease θ if derivative is positive.

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

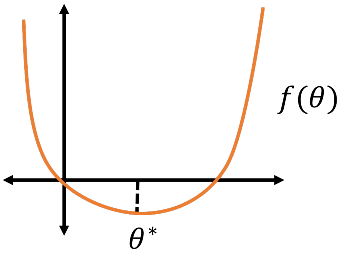
$$(1-\lambda) \cdot f(\vec{\theta}_1) + \lambda \cdot f(\vec{\theta}_2) \geq f\left((1-\lambda) \cdot \vec{\theta}_1 + \lambda \cdot \vec{\theta}_2\right)$$



CONVEXITY

Corollary: A function $f : \mathbb{R} \rightarrow \mathbb{R}$ is convex iff, for any $\theta_1, \theta_2 \in \mathbb{R}$:

$$\text{“slope between } f(\theta_1) \text{ and } f(\theta_2)\text{”} = \frac{f(\theta_2) - f(\theta_1)}{\theta_2 - \theta_1} \geq f'(\theta_1)$$



Corollary: A function $f : \mathbb{R} \rightarrow \mathbb{R}$ is convex iff, for any $\theta_1, \theta_2 \in \mathbb{R}$:

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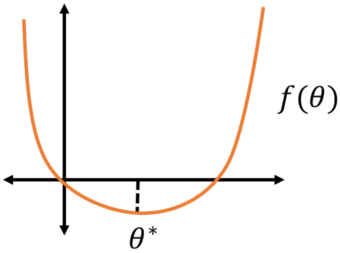
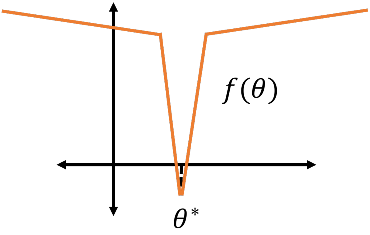
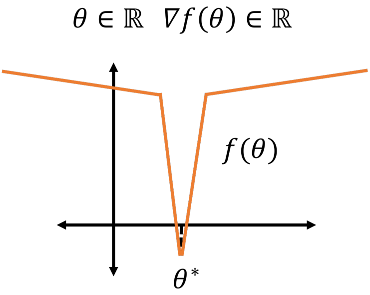
More generally, a function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is convex if and only if, for any $\vec{\theta}_1, \vec{\theta}_2 \in \mathbb{R}^d$: $f(\vec{\theta}_2) - f(\vec{\theta}_1) \geq \vec{\nabla} f(\vec{\theta}_1)^T \left(\vec{\theta}_2 - \vec{\theta}_1\right)$



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



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



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For fast convergence, need to assume that the function is Lipschitz, i.e., size of gradient $\|\vec{\nabla} f(\vec{\theta})\|_2$ is bounded. We'll assume

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

Gradient Descent analysis for convex, Lipschitz functions.

Assume that:

- f is convex.
- f is G Lipschitz, i.e., $\|\vec{\nabla} f(\vec{\theta})\|_2 \leq G$ for all $\vec{\theta}$.
- $\|\vec{\theta}_1 - \vec{\theta}_*\|_2 \leq R$ 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 $i = 1, \ldots, t-1$
  - $\vec{\theta}_{i+1} = \vec{\theta}_i - \eta \nabla f(\vec{\theta}_i)$
- Return $\hat{\theta} = \arg\min_{\vec{\theta}_1, \ldots \vec{\theta}_t} f(\vec{\theta}_i)$.

Theorem: For convex G-Lipschitz function $f : \mathbb{R} \to \mathbb{R}$, GD run with $t \geq \frac{R^2 G^2}{\epsilon^2}$ iterations, $\eta = \frac{R}{G\sqrt{t}}$, and starting point within R of θ_*, outputs $\hat{\theta}$ satisfying $f(\hat{\theta}) \leq f(\theta_*) + \epsilon$.

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- Substituting $\theta_{i+1} = \theta_i - \eta f'(\theta_i)$ and letting $a_i = \theta_i - \theta_*$ gives:

$$a_{i+1}^2 = (\theta_{i+1} - \theta_*)^2 = (a_i - \eta f'(\theta_i))^2 = a_i^2 - 2\eta f'(\theta_i) a_i + (\eta f'(\theta_i))^2$$

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- Rearrange and use convexity to show:

$$f(\theta_i) - f(\theta_*) \leq f'(\theta_i)a_i = \frac{1}{2\eta}\left(a_i^2 - a_{i+1}^2\right) + \eta(f'(\theta_i))^2/2$$

GD ANALYSIS PROOF

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- Summing over i and using the fact $|f'(\theta_i)| \leq G$,

$$\frac{1}{t}\sum_{i=1}^t \left(f(\theta_i) - f(\theta_*)\right) \leq \left(\frac{1}{2t\eta}\sum_{i=1}^t (a_i^2 - a_{i+1}^2)\right) + \frac{\eta G^2}{2} \leq \frac{a_1^2}{2t\eta} + \frac{\eta G^2}{2}$$

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- Using $a_1^2 \leq R^2$ and $f(\hat{\theta}) - f(\theta^*) \leq \frac{1}{t}\sum_{i=1}^{t}\left(f(\theta_i) - f(\theta_*)\right)$

$$f(\hat{\theta}) \leq f(\theta^*) + \frac{R^2}{2t\eta} + \frac{\eta G^2}{2} \leq f(\theta^*) + \epsilon$$

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Theorem: For convex G-Lipschitz function $f : \mathbb{R}^d \to \mathbb{R}$, 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 $f(\hat{\theta}) \leq f(\vec{\theta}_*) + \epsilon$.

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$$\begin{aligned}
\|\vec{\theta}_{i+1} - \vec{\theta}_*\|_2^2 &= \|\vec{\theta}_i - \eta \vec{\nabla} f(\vec{\theta}_i) - \vec{\theta}_*\|_2^2 \\
&= \|\vec{\theta}_i - \vec{\theta}_*\|_2^2 - 2\eta \vec{\nabla} f(\vec{\theta}_i)^T(\vec{\theta}_i - \vec{\theta}_*) + \|\eta \vec{\nabla} f(\theta_i)\|_2^2
\end{aligned}$$

using fact $\|a + b\|_2^2 = \|a\|_2^2 + 2a^T b + \|b\|_2^2$.

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\|\vec{\theta}_{i+1} - \vec{\theta}_*\|_2^2 &= \|\vec{\theta}_i - \eta\vec{\nabla} f(\vec{\theta}_i) - \vec{\theta}_*\|_2^2 \\
&= \|\vec{\theta}_i - \vec{\theta}_*\|_2^2 - 2\eta\vec{\nabla} f(\vec{\theta}_i)^T(\vec{\theta}_i - \vec{\theta}_*) + \|\eta\vec{\nabla} f(\theta_i)\|_2^2
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using fact $\|a+b\|_2^2 = \|a\|_2^2 + 2a^Tb + \|b\|_2^2$. Since $\|\eta\vec{\nabla} f(\vec{\theta}_i)\|_2^2 \leq \eta^2 G^2$,

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

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Proof of Step 2:

$$
\begin{aligned}
\sum_{i=1}^{t} f(\vec{\theta}_i) - f(\vec{\theta}_*) &\leq \frac{t\eta G^2}{2} + \frac{1}{2\eta}\sum_{i=0}^{t-1}\left(\|\vec{\theta}_i - \vec{\theta}_*\|_2^2 - \|\vec{\theta}_{i+1} - \vec{\theta}_*\|_2^2\right) \\
&= \frac{t\eta G^2}{2} + \frac{1}{2\eta}\|\vec{\theta}_0 - \vec{\theta}_*\|_2^2 \leq \frac{t\eta G^2}{2} + \frac{R^2}{2\eta}
\end{aligned}
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Theorem: For convex G-Lipschitz function $f : \mathbb{R}^d \to \mathbb{R}$, 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 $f(\hat{\theta}) \leq f(\vec{\theta}_*) + \epsilon$.

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Theorem: For convex G-Lipschitz function $f : \mathbb{R}^d \rightarrow \mathbb{R}$, 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 $f(\hat{\theta}) \leq f(\vec{\theta}_*) + \epsilon$.

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- Result follows since $\frac{1}{t}\sum_{i=1}^{t} f(\vec{\theta}_i) \geq f(\hat{\theta})$.

CONSTRAINED CONVEX OPTIMIZATION

Often want to perform convex optimization with convex constraints.

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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 $\lambda \in [0, 1]$: $(1 - \lambda)\vec{\theta}_1 + \lambda \cdot \vec{\theta}_2 \in \mathcal{S}$

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

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

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

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

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

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

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PROJECTED GRADIENT DESCENT ANALYSIS

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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.