COMPSCI 514: Algorithms for Data Science

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Lecture 22

Logistics

- Problem Set 4 due Friday at 11:59pm.
- Final exam is next Tuesday 5/12, 1-3pm in the lecture hall.
- Study guide and review material has been posted.
- Thursday's class will be dedicated to exam review.
- I will hold additional exam review office hours **Monday 5/11, 1:30-2:30pm**.
- Please fill out SRTIs for this class!

Summary

Last Class:

- Analysis of gradient descent for convex and Lipschitz functions.

This Class:

- Direct extension to gradient descent to constrained optimization via projected gradient descent.
- Analysis for convex functions and convex constraint sets.
- Online optimization and online gradient descent.
- Application to analysis of stochastic gradient descent, for gradient descent at scale.

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

Projection Function

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.

Gradient Descent at Scale: Online and Stochastic GD

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:

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

The gradient of $L(\vec{\theta}, \mathbf{X})$ has one component per data point so can be very expensive to compute.

Solution: Update using just a single data point, or a small batch of data points per iteration.

- If the data point is chosen uniformly at random, the sampled gradient is correct in expectation.

$$\vec{\nabla} L(\vec{\theta}, \mathbf{X}) = \sum_{i=j}^{n} \vec{\nabla} \ell(M_{\vec{\theta}}(\vec{x}_j), y_j) \rightarrow \mathbb{E}_{j \sim [n]}[\vec{\nabla} \ell(M_{\vec{\theta}}(\vec{x}_j), y_j)] = \frac{1}{n} \cdot \vec{\nabla} L(\vec{\theta}, \mathbf{X}).$$

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

Online Gradient Descent

SGD is closely related to online gradient descent.

In reality many learning problems are online.

- Websites optimize ads or recommendations to show users, given continuous feedback from these users.
- Spam filters are incrementally updated and adapt as they see more examples of spam over time.
- Face recognition systems, other classification systems, learn from mistakes over time.

Want to minimize some global loss $L(\vec{\theta}, \mathbf{X})$, when data points are presented in an online fashion $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n$ (like in streaming algorithms)

Will view SGD as a special case: when data points are presented (by design) in a random order.

Online Optimization Formal Setup

Online Optimization: In place of a single function f, we see a different objective function at each step:

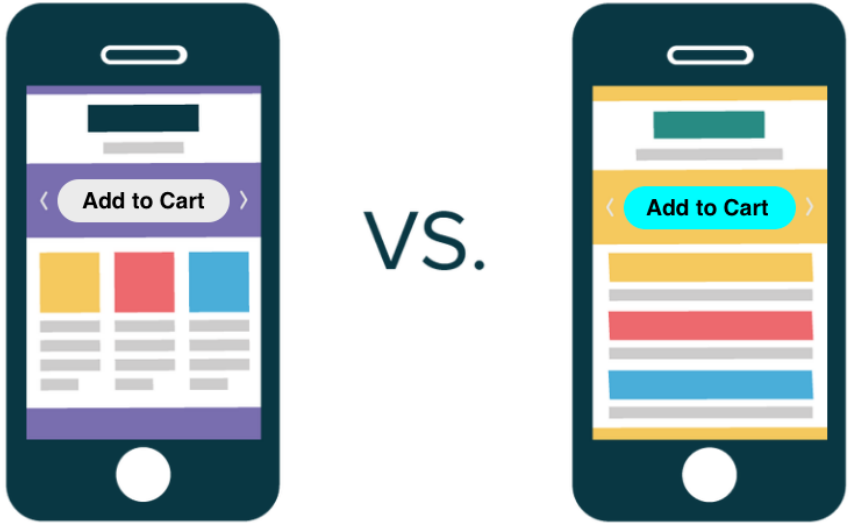
$$f_1, \ldots, f_t : \mathbb{R}^d \to \mathbb{R}$$

- At each step, first pick (play) a parameter vector $\vec{\theta}^{(i)}$.
- Then are told f_i and incur cost $f_i(\vec{\theta}^{(i)})$.
- **Goal:** Minimize total cost $\sum_{i=1}^{t} f_i(\vec{\theta}^{(i)})$.

No assumptions on how $f_1, \ldots, f_t$ are related to each other!

Online Optimization Example

UI design via online optimization.



- Parameter vector $\vec{\theta}^{(i)}$: some encoding of the layout at step i.
- Functions $f_1, \ldots, f_t$: $f_i(\vec{\theta}^{(i)}) = 1$ if user does not click 'add to cart' and $f_i(\vec{\theta}^{(i)}) = 0$ if they do click.
- Want to maximize number of purchases. I.e., minimize $\sum_{i=1}^{t} f_i(\vec{\theta}^{(i)})$

Online Optimization Example

Home pricing tools.

linear model

$\langle \vec{x}, \vec{\theta} \rangle$

$\$275{,}000$

$\vec{x} = [\#baths, \#beds, \#floors \ldots]$

- Parameter vector $\vec{\theta}^{(i)}$: coefficients of linear model at step i.
- Functions $f_1, \ldots, f_t$: $f_i(\vec{\theta}^{(i)}) = (\vec{\theta}^{(i)} - price_i)^2$ revealed when $home_i$ is listed or sold.
- Want to minimize total squared error $\sum_{i=1}^{t} f_i(\vec{\theta}^{(i)})$ (same as classic least squares regression).

Regret

In normal optimization, we seek $\hat{\theta}$ satisfying:

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

In online optimization we will ask for the same.

$$\sum_{i=1}^{t} f_i(\vec{\theta}^{(i)}) \leq \min_{\vec{\theta}} \sum_{i=1}^{t} f_i(\vec{\theta}) + \epsilon = \sum_{i=1}^{t} f_i(\vec{\theta}^{off}) + \epsilon$$

ϵ is called the regret.

- This error metric is a bit 'unfair'. Why?
- Comparing online solution to best fixed solution in hindsight. ϵ can be negative!

Online Gradient Descent

Assume that:

- $f_1, \ldots, f_t$ are all convex.
- Each f_i is G-Lipschitz (i.e., $\|\vec{\nabla} f_i(\vec{\theta})\|_2 \leq G$ for all $\vec{\theta}$.)
- $\|\vec{\theta}^{(1)} - \vec{\theta}^{off}\|_2 \leq R$ where $\theta^{(1)}$ is the first vector chosen.

Online Gradient Descent

- Set step size $\eta = \frac{R}{G\sqrt{t}}$.
- For $i = 1, \ldots, t$
  - Play $\vec{\theta}^{(i)}$ and incur cost $f_i(\vec{\theta}^{(i)})$.
  - $\vec{\theta}^{(i+1)} = \vec{\theta}^{(i)} - \eta \cdot \vec{\nabla} f_i(\vec{\theta}^{(i)})$

Online Gradient Descent Analysis

Theorem – OGD on Convex Lipschitz Functions: For convex G-Lipschitz $f_1, \ldots, f_t$, OGD initialized with starting point $\theta^{(1)}$ within radius R of θ^{off}, using step size $\eta = \frac{R}{G\sqrt{t}}$, has regret bounded by:

$$\left[\sum_{i=1}^{t} f_i(\theta^{(i)}) - \sum_{i=1}^{t} f_i(\theta^*)\right] \leq RG\sqrt{t}$$

Average regret goes to 0 and $t \to \infty$. 'Sublinear regret' or 'no regret' algorithm. No assumptions on how $f_1, \ldots, f_t$ are related to each other!

Step 1.1: For all i, $\nabla f_i(\theta^{(i)})^T(\theta^{(i)} - \theta^{off}) \leq \frac{\|\theta^{(i)} - \theta^{off}\|_2^2 - \|\theta^{(i+1)} - \theta^{off}\|_2^2}{2\eta} + \frac{\eta G^2}{2}$.

Convexity $\implies$ **Step 1:** For all i,

$$f_i(\theta^{(i)}) - f_i(\theta^{off}) \leq \frac{\|\theta^{(i)} - \theta^{off}\|_2^2 - \|\theta^{(i+1)} - \theta^{off}\|_2^2}{2\eta} + \frac{\eta G^2}{2}.$$

Online Gradient Descent Analysis

Theorem – OGD on Convex Lipschitz Functions: For convex G-Lipschitz $f_1, \ldots, f_t$, OGD initialized with starting point $\theta^{(1)}$ within radius R of θ^{off}, using step size $\eta = \frac{R}{G\sqrt{t}}$, has regret bounded by:

$$\left[\sum_{i=1}^{t} f_i(\theta^{(i)}) - \sum_{i=1}^{t} f_i(\theta^{off})\right] \leq RG\sqrt{t}$$

Step 1: For all i, $f_i(\theta^{(i)}) - f_i(\theta^{off}) \leq \frac{\|\theta^{(i)} - \theta^{off}\|_2^2 - \|\theta^{(i+1)} - \theta^{off}\|_2^2}{2\eta} + \frac{\eta G^2}{2} \implies$

$$\left[\sum_{i=1}^{t} f_i(\theta^{(i)}) - \sum_{i=1}^{t} f_i(\theta^{off})\right] \leq \sum_{i=1}^{t} \left(\frac{\|\theta^{(i)} - \theta^{off}\|_2^2 - \|\theta^{(i+1)} - \theta^{off}\|_2^2}{2\eta} + \frac{\eta G^2}{2}\right).$$

Stochastic Gradient Descent

Recall: Stochastic gradient descent is an efficient offline optimization method, seeking $\hat{\theta}$ with

$$f(\hat{\theta}) \leq \min_{\vec{\theta}} f(\vec{\theta}) + \epsilon = f(\vec{\theta}^*) + \epsilon.$$

Easily analyzed as a special case of online gradient descent!

Stochastic Gradient Descent

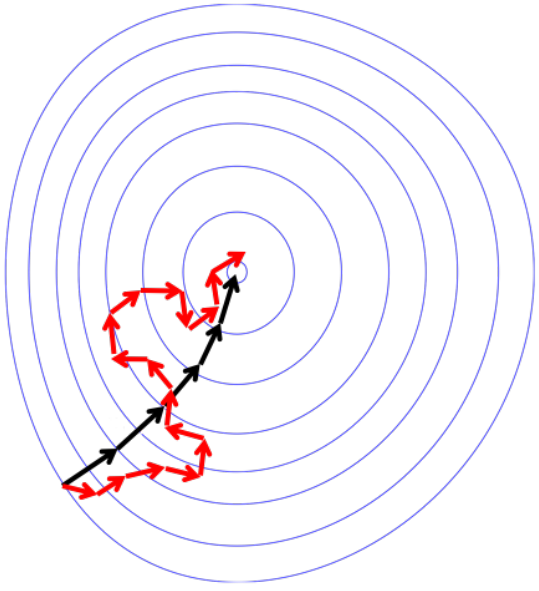
Assume that:

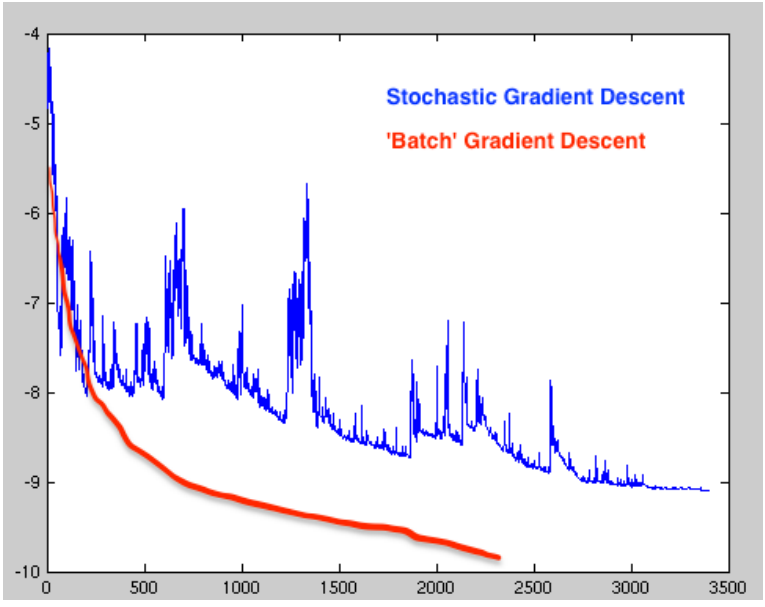
- f is convex and decomposable as $f(\vec{\theta}) = \sum_{j=1}^{n} f_j(\vec{\theta})$.
  - E.g., $L(\vec{\theta}, \mathbf{X}) = \sum_{j=1}^{n} \ell(M_{\vec{\theta}}(\vec{x}_j), y_j)$.
- Each f_j is $\frac{G}{n}$-Lipschitz (i.e., $\|\vec{\nabla} f_j(\vec{\theta})\|_2 \leq \frac{G}{n}$ for all $\vec{\theta}$.)
  - What does this imply about how Lipschitz f is?
- Initialize with $\theta^{(1)}$ satisfying $\|\vec{\theta}^{(1)} - \vec{\theta}^*\|_2 \leq R$.

Stochastic Gradient Descent

- Set step size $\eta = \frac{R}{G\sqrt{t}}$.
- For $i = 1, \ldots, t$
  - Pick random $j_i \in 1, \ldots, n$.
  - $\vec{\theta}^{(i+1)} = \vec{\theta}^{(i)} - \eta \cdot \vec{\nabla} f_{j_i}(\vec{\theta}^{(i)})$
- Return $\hat{\theta} = \frac{1}{t} \sum_{i=1}^{t} \vec{\theta}^{(i)}$.

Stochastic Gradient Descent





$\vec{\theta}^{(i+1)} = \vec{\theta}^{(i)} - \eta \cdot \vec{\nabla} f_{j_i}(\vec{\theta}^{(i)})$ vs. $\vec{\theta}^{(i+1)} = \vec{\theta}^{(i)} - \eta \cdot \vec{\nabla} f(\vec{\theta}^{(i)})$

Note that: $\mathbb{E}[\vec{\nabla} f_{j_i}(\vec{\theta}^{(i)})] = \frac{1}{n} \vec{\nabla} f(\vec{\theta}^{(i)})$.

Analysis extends to any algorithm that takes the gradient step in expectation (batch GD, randomly quantized, measurement noise, differentially private GD, etc.)

Stochastic Gradient Descent Analysis

Theorem – SGD on Convex Lipschitz Functions: SGD run with $t \geq \frac{R^2G^2}{\epsilon^2}$ iterations, $\eta = \frac{R}{G\sqrt{t}}$, and starting point within radius R of θ^*, outputs $\hat{\theta}$ satisfying: $\mathbb{E}[f(\hat{\theta})] \leq f(\theta^*) + \epsilon$.

Step 1: $f(\hat{\theta}) - f(\theta^*) \leq \frac{1}{t}\sum_{i=1}^{t}[f(\theta^{(i)}) - f(\theta^*)]$ (by convexity)

Step 2: $\mathbb{E}[f(\hat{\theta}) - f(\theta^*)] \leq \frac{n}{t} \cdot \mathbb{E}\left[\sum_{i=1}^{t}[f_{j_i}(\theta^{(i)}) - f_{j_i}(\theta^*)]\right]$.

Step 3: $\mathbb{E}[f(\hat{\theta}) - f(\theta^*)] \leq \frac{n}{t} \cdot \mathbb{E}\left[\sum_{i=1}^{t}[f_{j_i}(\theta^{(i)}) - f_{j_i}(\theta^{off})]\right]$.

Step 4: $\mathbb{E}[f(\hat{\theta}) - f(\theta^*)] \leq \frac{n}{t} \cdot \underbrace{R \cdot \frac{G}{n} \cdot \sqrt{t}}_{\text{OGD bound}} = \frac{RG}{\sqrt{t}}$.

SGD vs. GD

Stochastic gradient descent generally makes more iterations than gradient descent.

Each iteration is much cheaper (by a factor of n).

$$\vec{\nabla} \sum_{j=1}^{n} f_j(\vec{\theta}) \text{ vs. } \vec{\nabla} f_j(\vec{\theta})$$

SGD vs. GD

When $f(\vec{\theta}) = \sum_{j=1}^{n} f_j(\vec{\theta})$ and $\|\vec{\nabla} f_j(\vec{\theta})\|_2 \leq \frac{G}{n}$:

Theorem – SGD: After $t \geq \frac{R^2 G^2}{\epsilon^2}$ iterations outputs $\hat{\theta}$ satisfying:

$$\mathbb{E}[f(\hat{\theta})] \leq f(\theta^*) + \epsilon.$$

When $\|\vec{\nabla} f(\vec{\theta})\|_2 \leq \bar{G}$:

Theorem – GD: After $t \geq \frac{R^2 \bar{G}^2}{\epsilon^2}$ iterations outputs $\hat{\theta}$ satisfying:

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

$\|\vec{\nabla} f(\vec{\theta})\|_2 = \|\vec{\nabla} f_1(\vec{\theta}) + \ldots + \vec{\nabla} f_n(\vec{\theta})\|_2 \leq \sum_{j=1}^{n} \|\vec{\nabla} f_j(\vec{\theta})\|_2 \leq n \cdot \frac{G}{n} \leq G.$

When would this bound be tight?

Questions?