CS-GY 6763: Lecture 8
Second order conditions

NYU, Prof. Ainesh Bakshi

Gradient Descent

Conditions:

- **Convexity:** f is a convex function, $\mathcal{S}$ is a convex set.
- **Bounded Initial Distance:**

$$\|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2 \leq R$$

- **Bounded gradients (Lipschitz function)**:

$$\|\nabla f(\mathbf{x})\|_2 \leq G \text{ for all } \mathbf{x} \in \mathcal{S}.$$

Theorem (GD Convergence Bound)

(Projected) Gradient Descent outputs $\hat{\mathbf{x}}$ *with*

$$f(\hat{\mathbf{x}}) \leq \min_{\mathbf{x}\in\mathcal{S}} f(\mathbf{x}) + \epsilon, \quad \textit{after} \quad T = \frac{R^2 G^2}{\epsilon^2} \textit{ iterations.}$$

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$$\|\nabla f(x)\|_2 \leq G.$$

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- But in practice, the dependence on $1/\epsilon^2$ is pessimistic: gradient descent typically requires far fewer steps to reach ϵ error.
- Previous bounds only make a very weak first order assumption:

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- In practice, many functions satisfy stronger assumptions.

Second Order Conditions

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- We will give an appropriate generalization of these conditions to multi-dimensional functions shortly.
- **Takeaway:** Having either an upper or lower bound on the second derivative helps convergence. Having both helps a lot.

Improving Gradient Descent

Takeaway: Having either an upper and lower bound on the second derivative helps convergence. Having both helps a lot.

Number of iterations for ϵ error:

	G-Lipschitz	β-smooth
R bounded start	$O\left(\frac{G^2R^2}{\epsilon^2}\right)$	$O\left(\frac{\beta R^2}{\epsilon}\right)$
α-strong convex	$O\left(\frac{G^2}{\alpha\epsilon}\right)$	$O\left(\frac{\beta}{\alpha}\log(1/\epsilon)\right)$

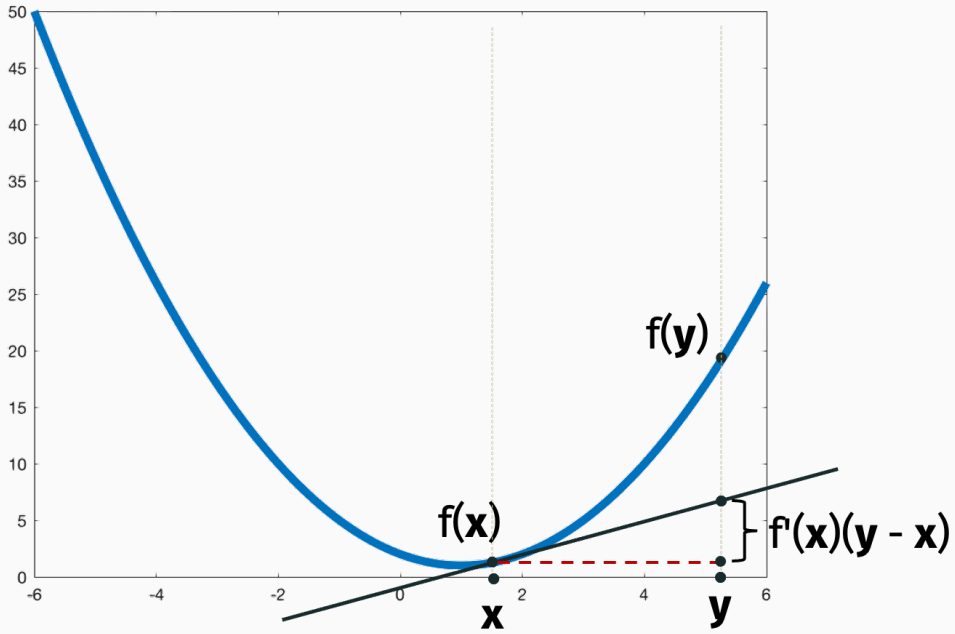
As we defined them so far, smoothness and strong convexity require f to be twice differentiable. On the other hand, gradient descent only requires first order differentiability.

Second Order Conditions

Equivalent conditions:

$$f''(x) \leq \beta \Rightarrow [f(y) - f(x)] - f'(x)(y-x) \leq \frac{\beta}{2}(y-x)^2$$

$$f''(x) \geq \alpha \Rightarrow [f(y) - f(x)] - f'(x)(y-x) \geq \frac{\alpha}{2}(y-x)^2$$



Recall: For all convex functions $[f(y) - f(x)] - f'(x)(y-x) \geq 0$.

Second Order Conditions

Proof that $f''(x) \leq \beta \Rightarrow [f(y) - f(x)] - f'(x)(y-x) \leq \frac{\beta}{2}(y-x)^2$:

Step 1: By FTC, $f(y) - f(x) = \int_x^y f'(t)\,dt$, so:

$$[f(y) - f(x)] - f'(x)(y-x) = \int_x^y [f'(t) - f'(x)]\,dt.$$

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Step 2: Apply FTC again: $f'(t) - f'(x) = \int_x^t f''(s)\,ds$, so:

$$\int_x^y [f'(t) - f'(x)]\,dt = \int_x^y \int_x^t f''(s)\,ds\,dt.$$

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Step 3: Since $f''(s) \leq \beta$:

$$\int_x^y \int_x^t f''(s)\,ds\,dt \leq \beta \int_x^y (t-x)\,dt = \frac{\beta}{2}(y-x)^2. \quad \square$$

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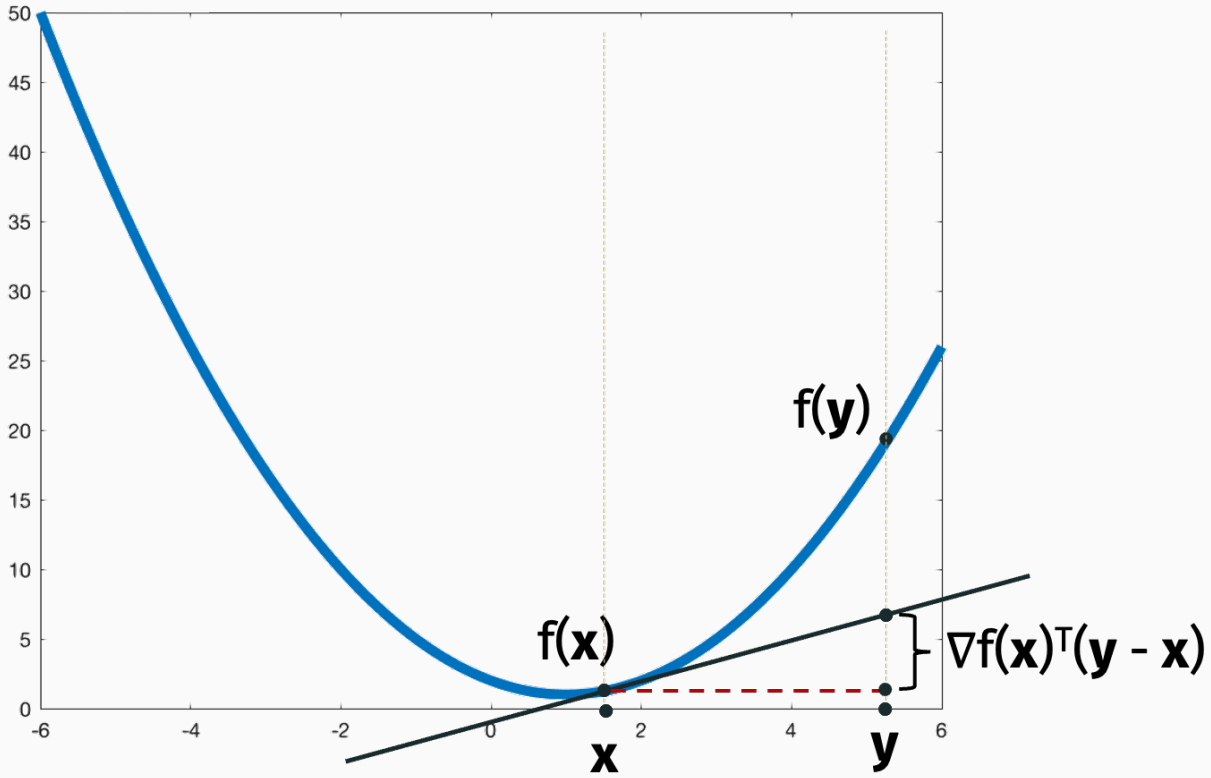
Proof for α-strongly convex is similar.

Multidimensional Generalization

A function is α-strongly convex and β-smooth if for all $\mathbf{x}$, $\mathbf{y}$:

$$\frac{\alpha}{2}\|\mathbf{y}-\mathbf{x}\|_2^2 \leq [f(\mathbf{y}) - f(\mathbf{x})] - \nabla f(\mathbf{x})^T(\mathbf{y}-\mathbf{x}) \leq \frac{\beta}{2}\|\mathbf{y}-\mathbf{x}\|_2^2$$



Convergence Guarantee

Theorem (GD Convergence for β-Smooth Functions)

Let f be a β-smooth convex function with $\|\mathbf{x}^* - \mathbf{x}^{(0)}\|_2 \leq R$. Running GD for T steps gives:

$$f\left(\mathbf{x}^{(T)}\right) - f\left(\mathbf{x}^*\right) \leq \frac{2\beta R^2}{T}.$$

Corollary: If $T = O\left(\frac{\beta R^2}{\epsilon}\right)$ then $f\left(\mathbf{x}^{(T)}\right) - f\left(\mathbf{x}^*\right) \leq \epsilon$.

Compare to $T = O\left(\frac{G^2 R^2}{\epsilon^2}\right)$ without a smoothness assumption.

Guaranteed Progress

Gradient descent for β-smooth functions:

- Select starting point $\mathbf{x}^{(0)}$, $\eta = 1/\beta$.
- For $i = 0, \ldots, T$:
  - $\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla f\left(\mathbf{x}^{(i)}\right)$
- Return $\hat{\mathbf{x}} = \arg\min_i f\left(\mathbf{x}^{(i)}\right)$.

Why do you think gradient descent might be faster when a function is β-smooth?

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Why do you think gradient descent might be faster when a function is β-smooth?

Intuitively, smoothness corresponds to the gradient being well-behaved everywhere.

Guaranteed Progress

With step size $\eta = \frac{1}{\beta}$, we have $\mathbf{x}^{(t+1)} - \mathbf{x}^{(t)} = -\frac{1}{\beta}\nabla f\left(\mathbf{x}^{(t)}\right)$.

Claim: $f\left(\mathbf{x}^{(t)}\right) - f\left(\mathbf{x}^{(t+1)}\right) \geq \frac{1}{2\beta}\|\nabla f\left(\mathbf{x}^{(t)}\right)\|_2^2$.

Proof:

1. Apply β-smoothness at $\mathbf{x}^{(t)}, \mathbf{x}^{(t+1)}$:

$$f\left(\mathbf{x}^{(t+1)}\right) \leq f\left(\mathbf{x}^{(t)}\right) + \nabla f\left(\mathbf{x}^{(t)}\right)^T\left(\mathbf{x}^{(t+1)} - \mathbf{x}^{(t)}\right) + \frac{\beta}{2}\|\mathbf{x}^{(t+1)} - \mathbf{x}^{(t)}\|_2^2.$$

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2. Substitute $\mathbf{x}^{(t+1)} - \mathbf{x}^{(t)} = -\frac{1}{\beta}\nabla f\left(\mathbf{x}^{(t)}\right)$:

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3. Rearranging: $f\left(\mathbf{x}^{(t)}\right) - f\left(\mathbf{x}^{(t+1)}\right) \geq \frac{1}{2\beta}\|\nabla f\left(\mathbf{x}^{(t)}\right)\|_2^2$. □

Telescoping Sum Proof

We have that $\frac{1}{2\beta}\|\nabla f\left(\mathbf{x}^{(t)}\right)\|_2^2 \leq f\left(\mathbf{x}^{(t)}\right) - f\left(\mathbf{x}^{(t+1)}\right)$. So:

$$\sum_{t=0}^{T-1} \frac{1}{2\beta}\|\nabla f\left(\mathbf{x}^{(t)}\right)\|_2^2 \leq f\left(\mathbf{x}^{(0)}\right) - f\left(\mathbf{x}^{(t)}\right)$$

$$\frac{1}{T}\sum_{t=0}^{T-1} \|\nabla f\left(\mathbf{x}^{(t)}\right)\|_2^2 \leq \frac{2\beta}{T}\left(f\left(\mathbf{x}^{(0)}\right) - f\left(\mathbf{x}^{*}\right)\right)$$

$$\min_t \|\nabla f\left(\mathbf{x}^{(t)}\right)\|_2^2 \leq \frac{2\beta}{T}\left(f\left(\mathbf{x}^{(0)}\right) - f\left(\mathbf{x}^{*}\right)\right)$$

Completing the Proof

For convex functions, we want to further prove that:

$$f\left(\hat{\mathbf{x}}\right) - f\left(\mathbf{x}^*\right) \leq \frac{2\beta R^2}{T}$$

Convex functions only have one stationary point: the global minimum $\mathbf{x}^*$. Ideally, we would argue that a near-stationary point is a near-minimizer. However, this isn't always the case!

Convergence Guarantee

Nevertheless, not to hard to obtain a proof from the progress condition. A concise version can be found on Page 15 in Garrigos and Gower's notes.

Theorem (GD convergence for β-smooth functions.)

Let f be a β smooth convex function and assume we have $\|\mathbf{x}^* - \mathbf{x}^{(1)}\|_2 \leq R$. If we run GD for T steps with $\eta = \frac{1}{\beta}$ we have:

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Note: This is not optimal! Can be improved to depend on $O(1/T^2)$ using a technique called acceleration.

Convergence Guarantee

What if f is both β-smooth and α-strongly convex?

Theorem (GD for β-smooth, α-strongly convex.)

Let f be a β-smooth and α-strongly convex function. If we run GD for T steps (with step size $\eta = \frac{1}{\beta}$) we have:

$$\|\mathbf{x}^{(T)} - \mathbf{x}^*\|_2^2 \leq e^{-T\frac{\alpha}{\beta}} \|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2^2$$

$\kappa = \frac{\beta}{\alpha}$ is called the "condition number" of f.

Smooth and Strongly Convex

Converting to more familiar form:

- Recall β-smoothness gives:

$$f(\mathbf{y}) - f(\mathbf{x}) - \nabla f(\mathbf{x})^T(\mathbf{y} - \mathbf{x}) \leq \frac{\beta}{2}\|\mathbf{x} - \mathbf{y}\|_2^2$$

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- Plug in $\mathbf{x} = \mathbf{x}^*$, $\mathbf{y} = \mathbf{x}^{(T)}$. Since $\nabla f(\mathbf{x}^*) = \mathbf{0}$:

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- Rearranging:
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- Rearranging:
$$\frac{2}{\beta}\left[f(\mathbf{x}^{(T)}) - f(\mathbf{x}^*)\right] \leq \|\mathbf{x}^{(T)} - \mathbf{x}^*\|_2^2$$

- We also assume $\|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2^2 \leq R^2$. Combined with
$$\|\mathbf{x}^{(T)} - \mathbf{x}^*\|_2^2 \leq e^{-T\alpha/\beta}\|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2^2$$
we get
$$f(\mathbf{x}^{(T)}) - f(\mathbf{x}^*) \leq \frac{\beta}{2}e^{-T\frac{\alpha}{\beta}}R^2$$

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Only depend on $\log(1/\epsilon)$ instead of on $1/\epsilon$ or $1/\epsilon^2$!

Can be further improved with acceleration to $O\left(\sqrt{\frac{\beta}{\alpha}}\log(\frac{R\beta}{\epsilon})\right)$!

Smooth, Strongly Convex Optimization

Later in class, we will prove the guarantee for the special case of:

$$f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$$

Goal: Get some of the key ideas across, introduces important concepts like the Hessian, and show the connection between conditioning and linear algebra.

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Rest of Today: online gradient descent and stochastic gradient descent.

Online and Stochastic Gradient Descent

- Basics of Online Learning + Optimization.

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- Introduction to Regret Analysis.

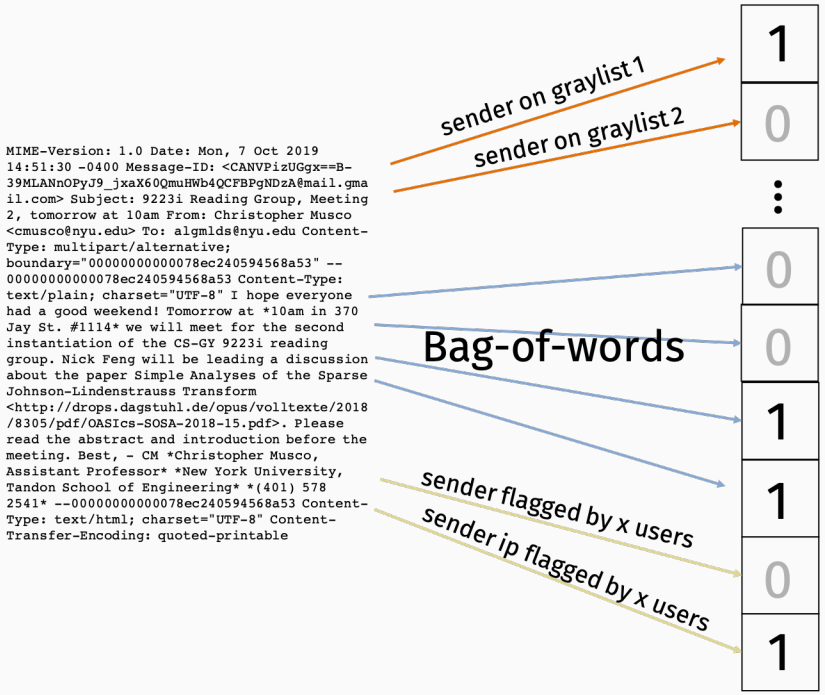
Online and Stochastic Gradient Descent

- Basics of Online Learning + Optimization.
- Introduction to Regret Analysis.
- Application to analyzing Stochastic Gradient Descent.

Original motivation for online learning: Often need to train machine learning models on constantly updating/changing data. Do not want to restart from scratch.

Example

Machine learning based email spam filtering.



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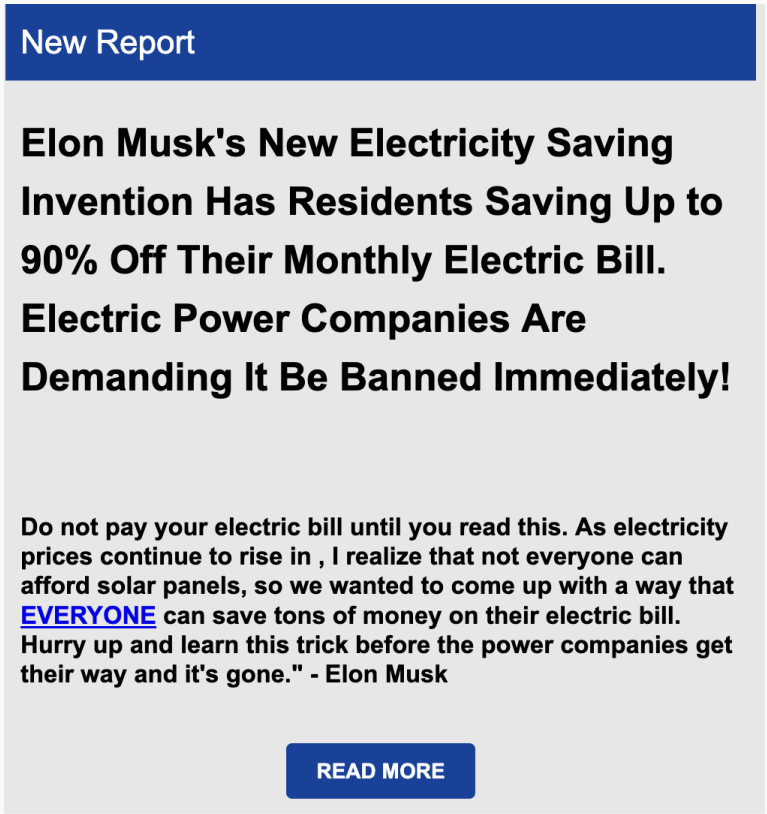

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Online Learning Framework

Choose some model $M_{\mathbf{x}}$ parameterized by parameters $\mathbf{x}$ and some loss function ℓ. At time steps $1, \ldots, T$, receive data vectors $\mathbf{a}^{(1)}, \ldots, \mathbf{a}^{(T)}$.

- At each time step, we pick ("play") a parameter vector $\mathbf{x}^{(i)}$.

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- At each time step, we pick ("play") a parameter vector $\mathbf{x}^{(i)}$.
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For example, for a regression problem we might use the ℓ_2 loss:

$$\ell(\mathbf{x}^{(i)}, \mathbf{a}^{(i)}, y^{(i)}) = \left(M_{\mathbf{x}^{(i)}}(\mathbf{a}_i) - y^{(i)}\right)^2.$$

For classification, we could use logistic/cross-entropy loss.

Online Optimization

Abstraction as optimization problem: Instead of a single objective function f, we have a unknown function $f_1, \ldots, f_T : \mathbb{R}^d \to \mathbb{R}$ for each time step.

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We make no assumptions that $f_1, \ldots, f_T$ are related to each other at all!

Regret Bound

In offline optimization, we wanted to find $\hat{\mathbf{x}}$ satisfying $f(\hat{\mathbf{x}}) \leq \min_{\mathbf{x}} f(\mathbf{x}) + \epsilon$. We ask for something similar here.

Objective: Choose $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(T)}$ so that:

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We typically want ϵ to grow sublinearly in T.

Regret Bound

Regret compares to the best fixed solution in hindsight.

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Exercise: Argue that the following is impossible to achieve:

$$\sum_{i=1}^{T} f_i\left(\mathbf{x}^{(i)}\right) \leq \left[\sum_{i=1}^{T} \min_{\mathbf{x}} f_i\left(\mathbf{x}\right)\right] + \epsilon.$$

Hard Example for Online Optimization

Convex functions:

$$f_1(x) = |x - h_1|$$

$$\vdots$$

$$f_T(x) = |x - h_T|$$

where $h_1, \ldots, h_T$ are i.i.d. uniform $\{0, 1\}$.

$$\mathrm{RHS} = \sum_{i=1}^{T} \min_{\mathbf{x_i}} f_i(\mathbf{x_i}) = 0 \qquad \text{by setting } x_i = h_i\,.$$

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$$\text{LHS} = \mathbb{E}\left[\sum_{i=1}^{T} f_i(\mathbf{x}^{(i)})\right] = \sum_{i=1}^{T} \frac{1}{2}\|0 - \mathbf{x}^{(i)}\| + \frac{1}{2}\|1 - \mathbf{x}^{(i)}\| \geq \frac{T}{2}$$

Regret Bounds

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Beautiful balance:

- Either $f_1, \ldots, f_T$ are similar or changing slowly, so we can learn/predict f_i from earlier functions.

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- Or we live somewhere in the middle.

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- Choose $\mathbf{x}^{(1)}$ and η.

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Only requires calculating gradient at one data point in each step

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$\mathbf{x}^* = \arg\min_{\mathbf{x}} \sum_{i=1}^{T} f_i(\mathbf{x})$ (the offline optimum)

Assume:

- $f_1, \ldots, f_T$ are all convex.
- Each is G-Lipschitz: for all $\mathbf{x}$, i, $\|\nabla f_i(\mathbf{x})\|_2 \leq G$.
- Starting radius: $\|\mathbf{x}^* - \mathbf{x}^{(1)}\|_2 \leq R$.

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Online Gradient Descent Analysis

Theorem (OGD Regret Bound)

If the conditions of the previous slide hold, then after T steps,

$$\epsilon = \left[\sum_{i=1}^{T} f_i\left(\mathbf{x}^{(i)}\right)\right] - \left[\sum_{i=1}^{T} f_i\left(\mathbf{x}^{*}\right)\right] \leq RG\sqrt{T}.$$

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- Average regret is bounded by $\frac{\epsilon}{T} \leq \frac{RG}{\sqrt{T}} \to 0$ as $T \to \infty$.
- All this with no assumptions on how $f_1, \ldots, f_T$ relate to each other — they could even be chosen **adversarially**.

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Claim 1: For all $i = 1, \ldots, T$,

$$f_i(\mathbf{x}^{(i)}) - f_i(\mathbf{x}^*) \leq \frac{\|\mathbf{x}^{(i)} - \mathbf{x}^*\|_2^2 - \|\mathbf{x}^{(i+1)} - \mathbf{x}^*\|_2^2}{2\eta} + \frac{\eta G^2}{2}$$

(We proved this by just plugging in $\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla f_i(\mathbf{x}^{(i)})$)

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$$\sum_{i=1}^{T} \left[f_i(\mathbf{x}^{(i)}) - f_i(\mathbf{x}^*)\right] \leq \frac{\|\mathbf{x}^{(1)} - \mathbf{x}^*\|_2^2 - \|\mathbf{x}^{(T)} - \mathbf{x}^*\|_2^2}{2\eta} + \frac{T\eta G^2}{2}$$

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&\leq \frac{R^2}{2\eta} + \frac{T\eta G^2}{2} \\
&\leq RG\sqrt{T} \quad \left(\text{recall } \eta = \frac{R}{G\sqrt{T}}\right)
\end{aligned}$$

Stochastic Gradient Descent (SGD)

Efficient offline optimization method for functions f with finite sum structure:

$$f(\mathbf{x}) = \sum_{i=1}^{n} f_i(\mathbf{x}).$$

Goal: find $\hat{\mathbf{x}}$ such that $f(\hat{\mathbf{x}}) \leq f(\mathbf{x}^*) + \epsilon$.

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- The most widely used optimization algorithm in modern machine learning.

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- The most widely used optimization algorithm in modern machine learning.
- Easily analyzed as a special case of online gradient descent!

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Recall the machine learning setup. In empirical risk minimization, we can typically write:

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$$f(\mathbf{x}) = \sum_{i=1}^{n} (\mathbf{x}^T \mathbf{a}^{(i)} - y^{(i)})^2$$

By linearity, $\nabla f(\mathbf{x}) = \sum_{i=1}^{n} \nabla f_i(\mathbf{x}) = \sum_{i=1}^{n} 2(\mathbf{x}^T \mathbf{a}^{(i)} - y^{(i)}) \cdot \mathbf{a}^{(i)}$.

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Key Idea: Compute only one term in the sum, chosen at random

Stochastic Gradient Descent

Key Idea: Use a random approximate gradient in place of the actual gradient

Pick random $j \in 1, \ldots, n$ and update $\mathbf{x}$ using $\nabla f_j(\mathbf{x})$:

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Trade slower convergence for cheaper iterations.

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Stochastic first-order oracle for $f(\mathbf{x}) = \sum_{j=1}^{n} f_j(\mathbf{x})$:

- **Function Query:** For any chosen $j, \mathbf{x}$, return $f_j(\mathbf{x})$
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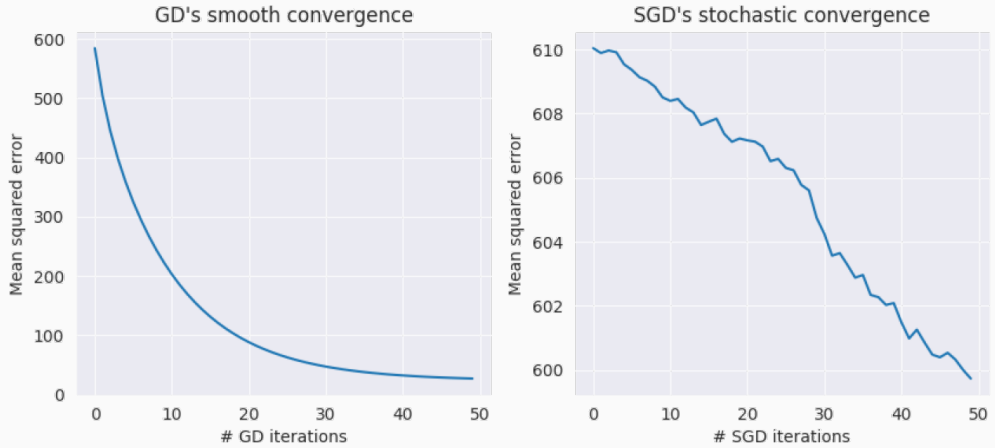
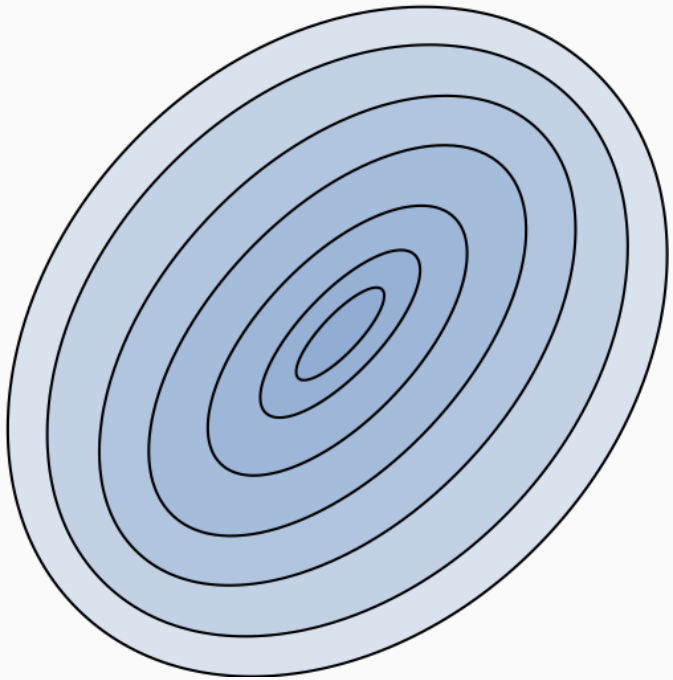
- Return $\hat{\mathbf{x}} = \frac{1}{T} \sum_{i=1}^{T} \mathbf{x}^{(i)}$.

visualizing SGD





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- Choose $\mathbf{x}^{(1)}$, steps T, step size $\eta = \frac{R}{G'\sqrt{T}}$.

Stochastic Gradient Descent

Assume:

- Finite sum structure: $f(\mathbf{x}) = \sum_{i=1}^{n} f_i(\mathbf{x})$, with $f_1, \ldots, f_n$ all convex.
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- Return $\hat{\mathbf{x}} = \frac{1}{T}\sum_{i=1}^{T} \mathbf{x}^{(i)}$.

View as online gradient descent run on function sequence $f_{j_1}, \ldots, f_{j_T}$.

Stochastic Gradient Descent Bound

Claim (SGD Convergence)

After $T = \frac{R^2 G'^2}{\epsilon^2}$ *iterations:*

$$\mathbb{E}\left[f\left(\hat{\mathbf{x}}\right) - f\left(\mathbf{x}^*\right)\right] \leq \epsilon.$$

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3. Jensen's inequality.

Jensen's Inequality

For a convex function f and points $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(t)}$:

$$f\left(\frac{1}{t}\sum_{k=1}^{t}\mathbf{x}^{(k)}\right) \leq \frac{1}{t}\sum_{k=1}^{t} f\left(\mathbf{x}^{(k)}\right)$$

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In other words: the function of the average is at most the average of the function.

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This is a generalization of

$$f\left(\frac{1}{2}x + \frac{1}{2}y\right) \leq \frac{1}{2}f(x) + \frac{1}{2}f(y)$$

Stochastic Gradient Descent Analysis

Claim (SGD Convergence)

Recall, $\hat{\mathbf{x}} = \frac{1}{T}\sum_{i=1}^{T}\mathbf{x}^{(i)}$. *After* $T = \frac{R^2 G'^2}{\epsilon^2}$ *iterations:*

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Claim 1: Cost of average iterate is bounded by average cost of the iterates.

$$f\left(\hat{\mathbf{x}}\right) - f\left(\mathbf{x}^*\right) \leq \frac{1}{T}\sum_{i=1}^{T}\left[f\left(\mathbf{x}^{(i)}\right) - f\left(\mathbf{x}^*\right)\right]$$

Prove using Jensen's Inequality:

$$f\left(\frac{1}{T}\sum_{i=1}^{T}\mathbf{x}^{(i)}\right) - \frac{1}{T}\sum_{i=1}^{T}f\left(\mathbf{x}^*\right) \leq \frac{1}{T}\sum_{i=1}^{T}f\left(\mathbf{x}^{(i)}\right) - \frac{1}{T}\sum_{i=1}^{T}f\left(\mathbf{x}^*\right)$$

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where $\mathbf{x}^{offline} = \arg\min_x \sum_{i=1}^{T} f_{j_i}(\mathbf{x})$. Thus, $\sum_{i=1}^{T} f_{j_i}(\mathbf{x}^{offline}) \leq \sum_{i=1}^{T} f_{j_i}(\mathbf{x}^*)$

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&\leq \frac{n}{T}\cdot\left(R\cdot\frac{G'}{n}\cdot\sqrt{T}\right) \qquad \text{(by OGD guarantee.)} \\
&\leq \frac{RG'}{\sqrt{T}} \leq \epsilon
\end{aligned}$$

Stochastic vs. Full Batch Gradient Descent

Number of iterations for error ϵ:

- **Gradient Descent**: $T = \frac{R^2 G^2}{\epsilon^2}$.
- **Stochastic Gradient Descent**: $T = \frac{R^2 G'^2}{\epsilon^2}$.

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So GD converges in fewer iterations than SGD.

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So GD converges in fewer iterations than SGD.

But for a fair comparison:

- SGD cost = (# of iterations) $\cdot\, O(1)$
- GD cost = (# of iterations) $\cdot\, O(n)$

Stochastic vs. Full Batch Gradient Descent

We always have $G \leq G'$. When it is much smaller, GD will perform better. When it is close to this upper bound, SGD will perform better.

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What is an extreme case where $G = G'$?

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What is an extreme case where $G = G'$?

- When all the f_i's are the same, i.e. is all the data points are identical
- SGD does better when there are lots of repetitions in the dataset

Stochastic vs. Full Batch Gradient Descent

What if each gradient $\nabla f_i(\mathbf{x})$ looks like a random vector in $\mathbb{R}^d$ with $\mathcal{N}(0,1)$ entries?

$$\mathbb{E}\left[\|\nabla f_i(\mathbf{x})\|_2^2\right] = d$$

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If you compare cost of GD vs SGD on such an instance, there will be no gain.

Stochastic vs. Full Batch Gradient Descent

Takeaway: SGD performs better when there is more structure or repetition in the data set.