# CS-GY 6763: Lecture 6 Online and Stochastic Gradient Decent

NYU Tandon School of Engineering, Prof. Christopher Musco

- Midterm in class next Tuesday. .
  - See Ed post.
  - If you have permission to take remotely, please email asap so I know who you are.
  - List of topics covered and practice problems are on the course webpage.
- Tomorrow in the reading group Hayden Edelson will present Estimating Sizes of Social Networks via Biased Sampling. See you there!
- Thanks to **Robert Ronan** for the presentation last week.

First Order Optimization: Given a function f and a constraint set S, assume we have:

- Function oracle: Evaluate  $f(\mathbf{x})$  for any  $\mathbf{x}$ .
- Gradient oracle: Evaluate  $\nabla f(\mathbf{x})$  for any  $\mathbf{x}$ .
- **Projection oracle**: Evaluate  $P_{\mathcal{S}}(\mathbf{x})$  for any  $\mathbf{x}$ .

**Goal:** Find  $\hat{\mathbf{x}} \in S$  such that  $f(\hat{\mathbf{x}}) \leq \min_{\mathbf{x} \in S} f(\mathbf{x}) + \epsilon$ .

# Projected gradient descent:

• Select starting point  $\underline{\mathbf{x}}^{(0)}$ , learning rate  $\eta$ .

• For 
$$i = 0, ..., T$$
:  

$$\chi^{(l+1)} = \mathbf{z} = \mathbf{x}^{(i)} - \eta \nabla f(\mathbf{x}^{(i)})$$
•  $\mathbf{x}^{(i+1)} = P_{\mathcal{S}}(\mathbf{z})$ 

• Return  $\hat{\mathbf{x}} = \arg\min_i f(\mathbf{x}^{(i)})$ .

Conditions for convergence:

- **Convexity:** f is a convex function, S is a convex set.
- · Bounded initial distance:

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

• Bounded gradients (Lipschitz function):

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

**Theorem:** Projected Gradient Descent returns  $\hat{\mathbf{x}}$  with  $f(\hat{\mathbf{x}}) \leq \min_{\mathbf{x} \in S} f(\mathbf{x}) + \epsilon$  after

$$T = \frac{R^2 G^2}{\epsilon^2}$$

iterations.

Convexity:

$$0 \leq [f(\mathbf{y}) - f(\mathbf{x})] - \nabla f(\mathbf{x})^{\mathsf{T}}(\mathbf{y} - \mathbf{x}) \leq 0$$

 $\alpha$ -strong-convexity and  $\beta$ -smoothness:  $\alpha \leq \beta'(x) \leq \beta$ 

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

Number of iterations for  $\epsilon$  error:

	G- <u>Lipschit</u> z	eta-smooth
R bounded start	$O\left(\frac{G^2R^2}{\epsilon^2}\right)$	$O\left(\frac{\beta R^2}{\epsilon}\right)$
lpha-strong convex	$O\left(\frac{G^2}{\alpha\epsilon}\right)$	$O\left(\frac{\beta}{\alpha}\log(1/\epsilon)\right)$

#### CONVERGENCE GUARANTEE

#### Theorem (GD for $\beta$ -smooth, $\alpha$ -strongly convex.)

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

$$\frac{\|\mathbf{x}^{(T)} - \mathbf{x}^*\|_2^2}{\leq e^{-(T^{(T)})} |\mathbf{x}^{(0)} - \mathbf{x}^*\|_2^2} \qquad \mathbf{j} \in \frac{B}{2} |\mathbf{x}^{(1)} \times \mathbf{x}^*|_2^2}{\leq e^{-(T^{(T)})} \cdot \mathbf{x}^*|_2^2} \qquad \mathbf{j} \in \frac{B}{2} |\mathbf{x}^{(1)} \cdot \mathbf{x}^*|_2^2$$

Corollary: If  $T = O\left(\frac{\beta}{\alpha}\log(R\beta/\epsilon)\right)$  we have:  $f(\mathbf{x}^{(T)}) - f(\mathbf{x}^*) \le \epsilon$ 

We will prove this in the special case of

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

where  $\mathbf{x} \in \mathbb{R}^d$ ,  $\mathbf{A} \in \mathbb{R}^{n \times d}$ ,  $\mathbf{b} \in \mathbb{R}^n$ .

Let *f* be a twice differentiable function from  $\mathbb{R}^d \to \mathbb{R}$ . Let the **Hessian**  $\mathbf{H} = \nabla^2 f(\mathbf{x})$  contain all of its second derivatives at a point  $\mathbf{x}$ . So  $\mathbf{H} \in \mathbb{R}^{d \times d}$ . We have:

$$\mathsf{H}_{i,j} = \left[\nabla^2 f(\mathsf{x})\right]_{i,j} = \underbrace{\partial^2 f}_{\partial x_i x_j}.$$

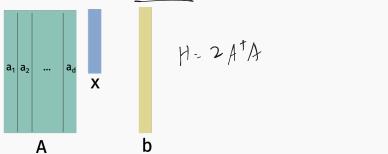
For vector **x**, **v**:

$$\nabla f(\mathbf{x} + t\mathbf{v}) \approx \nabla f(\mathbf{x}) + t \left[\nabla^2 f(\mathbf{x})\right] \mathbf{v}.$$

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$$\mathsf{H}_{i,j} = \left[\nabla^2 f(\mathsf{x})\right]_{i,j} = \frac{\partial^2 f}{\partial x_i x_j}$$

**Example:** Let  $f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$ . Recall that  $\nabla f(\mathbf{x}) = 2\mathbf{A}^T(\mathbf{A}\mathbf{x} - \mathbf{b})$ .



**Claim:** If *f* is twice differentiable, then it is convex if and only if the matrix  $\mathbf{H} = \nabla^2 f(\mathbf{x})$  is positive semidefinite for all  $\mathbf{x}$ .

# Definition (Positive Semidefinite (PSD))

This is a natural notion of "positivity" for symmetric matrices. To denote that **H** is PSD we will typically use "Loewner order" notation (\succeq in LaTex):

**Claim:** If *f* is twice differentiable, then it is convex if and only if the matrix  $\mathbf{H} = \nabla^2 f(\mathbf{x})$  is positive semidefinite for all  $\mathbf{x}$ .

## Definition (Positive Semidefinite (PSD))

A square, symmetric matrix  $\mathbf{H} \in \mathbb{R}^{d \times d}$  is <u>positive semidefinite</u> (PSD) for any vector  $\mathbf{y} \in \mathbb{R}^d$ ,  $\mathbf{y}^T \mathbf{H} \mathbf{y} \ge 0$ .

For the least squares regression loss function:  $f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$ ,  $\mathbf{H} = \nabla^2 f(\mathbf{x}) = 2\mathbf{A}^T \mathbf{A}$  for all  $\mathbf{x}$ .

We know that *H* is PSD because:

$$\mathbf{x}^{T}\mathbf{H}\mathbf{x} = 2\mathbf{x}^{T}\mathbf{A}^{T}\mathbf{A}\mathbf{x} = 2\|\mathbf{A}\mathbf{x}\|_{2}^{2} \ge 0.$$
$$\mathbf{x}^{T}\mathbf{A}^{T} = [\mathbf{A}\mathbf{x}]^{T} \qquad \mathbf{y} (\mathbf{A}\mathbf{x})^{T} (\mathbf{A}\mathbf{y}) = \mathbf{y}\|\mathbf{A}\mathbf{x}\|_{2}^{2}$$

#### THE LINEAR ALGEBRA OF CONDITIONING

If *f* is  $\beta$ -smooth and  $\alpha$ -strongly convex then at any point **x**,  $\mathbf{H} = \nabla^2 f(\mathbf{x}) \text{ satisfies:}$ 

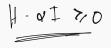
$$\alpha \mathbf{I}_{d \times d} \preceq \mathbf{H} \preceq \beta \mathbf{I}_{d \times d}$$

where  $I_{d \times d}$  is a  $d \times d$  identity matrix.

This is the natural matrix generalization of the statement for scalar valued functions:

$$\alpha \leq f''(\mathbf{X}) \leq \beta.$$

#### SMOOTH AND STRONGLY CONVEX HESSIAN



$$\begin{bmatrix} \lambda d_{1}^{\vee} - \alpha & 0 \\ 0 & \lambda & d_{2}^{\vee} - \alpha \end{bmatrix}$$

$$\alpha \mathbf{I}_{d \times d} \preceq \mathbf{H} \preceq \beta \mathbf{I}_{d \times d}.$$

Equivalently for any **z**,

$$\alpha \|\mathbf{z}\|_2^2 \le \mathbf{z}^T \mathbf{H} \mathbf{z} \le \beta \|\mathbf{z}\|_2^2.$$

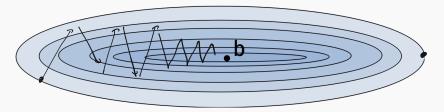
#### SIMPLE EXAMPLE

Let  $f(\mathbf{x}) = (|\mathbf{D}\mathbf{x} - \mathbf{b}||_2^2)$  where **D** is a diagaonl matrix. For now imagine we're in two dimensions:  $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ ,  $\mathbf{D} = \begin{bmatrix} d_1 & 0 \\ 0 & d_2 \end{bmatrix}$ .

What are  $\underline{\alpha, \beta}$  for this problem?

#### **GEOMETRIC VIEW**

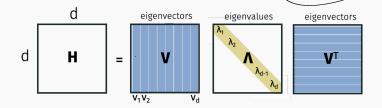
2= 6=1 hi stor. Level sets of  $\|\mathbf{Dx} - \mathbf{b}\|_2^2$  when  $d_1^2 = 1, d_2^2 = 1$ . - 11X-5112



Level sets of  $\|\underline{\mathbf{Dx}} - \mathbf{b}\|_2^2$  when  $d_1^2 = \frac{1}{3}, d_2^2 = 2$ .

#### EIGENDECOMPOSITION VIEW

Any symmetric matrix **H** has an <u>orthogonal</u>, real-valued eigendecomposition.



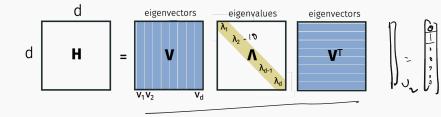
Here V is square and orthogonal, so  $V^T V = V V^T = I$ . And for each  $v_i$ , we have:

$$\mathsf{H}\underline{\mathsf{v}_{i}} = \lambda_{i}\mathsf{v}_{i}.$$

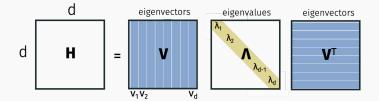
By definition, that's what makes  $\mathbf{v}_1, \ldots, \mathbf{v}_d$  eigenvectors.

#### EIGENDECOMPOSITION VIEW

Recall  $VV^{T} = V^{T}V = I$ .



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.

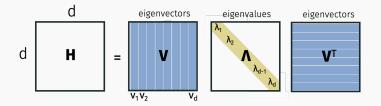


Claim:  $\alpha I \preceq H \preceq \beta I \Leftrightarrow \alpha \leq \lambda_d \leq ... \leq \lambda_1 \leq \beta$ .

$$H - \chi T > 0$$

$$V \wedge V^{T} - \alpha \vee V^{T} = V (\Lambda - 0 I) V^{T}$$

Recall  $VV^{T} = V^{T}V = I$ .



In other words, if we let  $\lambda_{max}(H)$  and  $\lambda_{min}(H)$  be the smallest and largest eigenvalues of H, then for all z we have:

$$\begin{split} \mathbf{z}^{\mathsf{T}}\mathbf{H}\mathbf{z} &\leq \lambda_{\mathsf{max}}(\mathbf{H}) \cdot \|\mathbf{z}\|^2 \\ \mathbf{z}^{\mathsf{T}}\mathbf{H}\mathbf{z} &\geq \lambda_{\mathsf{min}}(\mathbf{H}) \cdot \|\mathbf{z}\|^2 \end{split}$$

If the maximum eigenvalue of  $\mathbf{H} = \nabla^2 f(\mathbf{x}) = \beta$  and the minimum eigenvalue of  $\mathbf{H} = \nabla^2 f(\mathbf{x}) = \alpha$  then  $f(\mathbf{x})$  is  $\beta$ -smooth and  $\alpha$ -strongly convex.

$$\lambda_{\max}(\mathsf{H}) = \underline{\beta}$$
$$\lambda_{\min}(\mathsf{H}) = \alpha$$

#### POLYNOMIAL VIEW POINT

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

$$\|\mathbf{x}^{(T+1)} - \mathbf{x}^*\|_2 \le e^{-T/\kappa} \|\mathbf{x}^{(1)} - \mathbf{x}^*\|_2$$

$$\chi = 2^{h^{h}}$$
 Goal: Prove for  $f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_{2}^{2}$ .

Let  $\lambda_{\max} = \lambda_{\max}(\mathbf{A}^{\mathsf{T}}\mathbf{A})$ . Gradient descent update is:

$$\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \frac{1}{2\lambda_{\max}} 2\mathbf{A}^{\mathsf{T}} (\mathbf{A}\mathbf{x}^{(t)} - \mathbf{b})$$

#### ALTERNATIVE VIEW OF GRADIENT DESCENT

$$A^{+}(A \times^{+} - b) = 0 \qquad A^{+}A \times^{+} = A^{+}b \qquad A^{+}b = A^{+}A \times^{+}$$
Richardson Iteration view:  

$$A^{+}b = A^{+}A \times^{+}$$

$$A^{+}b = A^{+}A \times^{+}$$

$$X^{(t+1)} - x^{*} = \left(I - \frac{1}{\lambda_{\max}}A^{T}A\right) \left(\frac{x^{(t)} - x^{*}}{\lambda_{\max}}\right)$$

$$\chi^{(t+1)} - \chi^{*} = \chi^{(t)} - \frac{1}{\lambda_{\max}}A^{+}(A \times^{(t)} - b) - \chi^{+}$$

$$\chi^{(t+1)} - \chi^{*} = \chi^{(t)} - \frac{1}{\lambda_{\max}}A^{+}(A \times^{(t)} - b) - \chi^{+}$$

$$\chi^{(t+1)} - \chi^{*} = \left(I - \frac{1}{\lambda_{\max}}A^{+}A \times^{(t)} - \frac{1}{\lambda_{\max}}A^{+}A \times^{(t)} - \frac{1}{\lambda_{\max}}A^{+}A \times^{(t)}\right)$$

$$A^{+}A = V \Lambda V^{T} = \left(I - \frac{1}{\lambda_{\max}}A^{+}A\right) \left(\chi^{(t)} - \chi^{*}\right) \qquad 1 - \frac{\lambda_{\max}}{\lambda_{\max}}$$
What is the maximum eigenvalue of the symmetric matrix  

$$\left(I - \frac{1}{\lambda_{\max}}A^{T}A\right) = \frac{\lambda_{d}}{\lambda_{\max}} = \frac{\lambda_{\min}}{\lambda_{\max}} \text{ of } A^{T}A? \qquad V \Lambda V^{T}$$

$$X^{T} = \frac{\lambda_{1}}{\lambda_{\max}} = \frac{\lambda_{1}}{\lambda_{1}} =$$

#### UNROLLED GRADIENT DESCENT

#### UNROLLED GRADIENT DESCENT

$$(\mathbf{x}^{(T+1)} - \mathbf{x}^{*}) = \left(\mathbf{I} - \frac{1}{\lambda_{\max}}\mathbf{A}^{T}\mathbf{A}\right)^{T} (\mathbf{x}^{(1)} - \mathbf{x}^{*})$$

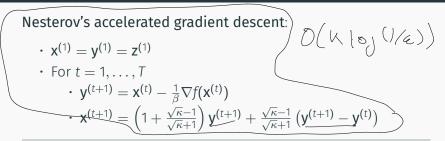
$$\mathcal{W} = \left(\mathbf{I} - \frac{1}{\lambda_{\max}} \mathbf{A}^{T}\mathbf{A}\right)^{T} = \mathbf{U} \mathbf{C} \mathbf{U}^{T}$$

$$\mathcal{W} = \left(\mathbf{U} - \frac{1}{\lambda_{\max}} \mathbf{A}^{T}\mathbf{A}\right)^{T} = \mathbf{U} \mathbf{C} \mathbf{U}^{T}$$

$$\mathbf{W} = \left(\mathbf{U} - \frac{1}{\lambda_{\max}} \mathbf{A}^{T}\mathbf{A}\right)^{T} = \left(\frac{1}{\lambda_{\max}} - \frac{1}{\lambda_{\max}} - \frac{1}{\lambda_{\max}$$

#### ACCELERATION

#### ACCELERATED GRADIENT DESCENT



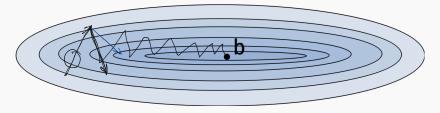
Theorem (AGD for  $\beta$ -smooth,  $\alpha$ -strongly convex.)

Let f be a  $\beta$ -smooth and  $\alpha$ -strongly convex function. If we run AGD for T steps we have:

$$f(\mathbf{x}^{(t)}) - f(\mathbf{x}^*) \le \kappa e^{-(t-1)\sqrt{\kappa}} \left[ f(\mathbf{x}^{(1)}) - f(\mathbf{x}^*) \right]$$

**Corollary:** If  $T = O(\sqrt{\kappa} \log(\kappa/\epsilon))$  achieve error  $\epsilon$ .

#### INTUITION BEHIND ACCELERATION



Level sets of  $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$ .

# Other terms for similar ideas:

- Momentum
- Heavy-ball methods

What if we look back beyond two iterates?

# BREAK

# Second part of class:

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

# Many machine learning problems are solved in an <u>online</u> setting with constantly changing data.

- Spam filters are incrementally updated and adapt as they see more examples of spam over time.
- Image classification systems learn from mistakes over time (often based on user feedback).
- Content recommendation systems adapt to user behavior and clicks (which may not be a good thing...)

EXAMPLE

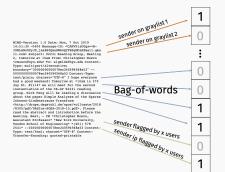
### Plant identification via iNaturalist app.

(California Academy of Science + National Geographic)



- When the app fails, image is classified via crowdsourcing (backed by huge network of amateurs and experts).
- Single model that is updated constantly, not retrained in batches.

#### ML based email spam/scam filtering.



Markers for spam change overtime, so model might change.

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Markers for spam change overtime, so model might change.

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

- At each time step, we pick ("play") a parameter vector  $\mathbf{x}^{(i)}$ .
- Make prediction  $\tilde{y}^{(i)} = M_{\mathbf{x}^{(i)}}(\mathbf{a}_{\mathbf{z}}^{(i)})$ .
- Then told true value or label  $y^{(i)}$ .
- Goal is to minimize cumulative loss:

$$y^{(r)} - M_x i_3(q^{(r)})$$

$$L = \sum_{i=1}^{n} \ell(\mathbf{x}^{(i)}, \mathbf{a}^{(i)}, \mathbf{y}^{(i)})$$

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For example, for a regression problem we might use the 
$$\ell_2$$
 loss:

$$\ell(\mathbf{x}^{(i)},\mathbf{a}^{(i)},y^{(i)}) = \left\lfloor \langle \mathbf{x}^{(i)},\mathbf{a}^{(i)} \rangle - y^{(i)} \right\rfloor^2.$$

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

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

- For time step  $i \in 1, \ldots, T$ , select vector  $\mathbf{x}^{(i)}$ .
- Observe  $f_i$  and pay cost  $f_i(\mathbf{x}^{(i)})$
- Goal is to minimize  $\sum_{i=1}^{T} f_i(\mathbf{x}^{(i)})$ .

We make <u>no assumptions</u> 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  $f(\hat{\mathbf{x}}) \leq \min_{\mathbf{x}} f(\mathbf{x})$ . Ask for a similar thing here.

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

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

Here  $\epsilon$  is called the regret of our solution sequence  $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(7)}$ .

Regret compares to the best fixed solution in hindsight.

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

It's very possible that  $\sum_{i=1}^{T} f_i(\mathbf{x}^{(i)}) < [\min_{\mathbf{x}} \sum_{i=1}^{T} f_i(\mathbf{x})]$ . Could we hope for something stronger?

Exercise: Argue that the following is impossible to achieve:

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

# Convex functions:

$$f_{1}(x) = |x - h_{1}| = |X|$$

$$\vdots = |x - 1|$$

$$f_{T}(x) = |x - h_{T}| = |X|$$
where  $h_{1}, \dots, h_{T}$  are i.i.d. uniform  $\{0, 1\}$ .
$$\begin{cases} f_{1}(x) = |x - h_{T}| \\ |x| \\ |x|$$

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

Beautiful balance:

- Either  $f_1, \ldots, f_T$  are similar, so we can learn predict  $f_i$  from earlier functions.
- Or  $f_1, \ldots, f_T$  are very different, in which case  $\min_{\mathbf{x}} \sum_{i=1}^T f_i(\mathbf{x})$  is large, so regret bound is easy to achieve.
- Or we live somewhere in the middle.

Online Gradient descent:

- Choose  $\mathbf{x}^{(1)}$  and  $\eta = \frac{R}{G\sqrt{T}}$ .
- For i = 1, ..., T:
  - Play  $\mathbf{x}^{(i)}$ .
  - Observe  $f_i$  and incur cost  $f_i(\mathbf{x}^{(i)})$ .

$$\cdot \mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla f_i(\mathbf{x}^{(i)})$$

If  $f_1, \ldots, f_T = f$  are all the same, this looks a lot like regular gradient descent. We update parameters using the gradient  $\nabla f$  at each step.

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

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

Online Gradient descent:

- Choose  $\mathbf{x}^{(1)}$  and  $\eta = \frac{R}{G\sqrt{T}}$ .
- For i = 1, ..., T:
  - Play  $\mathbf{x}^{(i)}$ .
  - Observe  $f_i$  and incur cost  $f_i(\mathbf{x}^{(i)})$ .
  - $\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} \eta \nabla f_i(\mathbf{x}^{(i)})$

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

Theorem (OGD Regret Bound) After T steps,  $\epsilon = \left[\sum_{i=1}^{T} f_i(\mathbf{x}^{(i)})\right] - \left[\sum_{i=1}^{T} f_i(\mathbf{x}^*)\right] \le \underline{RG}\sqrt{T}.$ 

Average regret overtime is bounded by  $\frac{\epsilon}{T} \leq \frac{RG}{\sqrt{T}}$ . Goes  $\rightarrow$  0 as  $T \rightarrow \infty$ .

All this with no assumptions on how  $f_1, \ldots, f_T$  relate to each other! They could have even been chosen adversarially – e.g. with  $f_i$  depending on our choice of  $\mathbf{x}_i$  and all previous choices.

Theorem (OGD Regret Bound) After T steps,  $\epsilon = \left[\sum_{i=1}^{T} f_i(\mathbf{x}^{(i)})\right] - \left[\sum_{i=1}^{T} f_i(\mathbf{x}^*)\right] \le RG\sqrt{T}.$ 

**Claim 1:** For all i = 1, ..., T,

$$f_{i}(\mathbf{x}^{(i)}) - f_{i}(\mathbf{x}^{*}) \leq \frac{\|\mathbf{x}^{(i)} - \mathbf{x}^{*}\|_{2}^{2} - \|\mathbf{x}^{(i+1)} - \mathbf{x}^{*}\|_{2}^{2}}{2\eta} + \frac{\eta G^{2}}{2}$$
Same proof as last class. Only uses convexity of  $f_{i}$ .)
$$f_{i}^{(i_{1})} = \chi^{*} \|_{\gamma}^{1} : \|\chi^{(i)} - \eta \forall f_{i}(\chi^{(i)}) - \chi^{*}\|_{\gamma}^{1} = \|\chi^{(i)} - \chi^{*}\|_{\gamma}^{1} : \|\chi^{(i)} - \chi^{*}\|_{\gamma}^{1} + \|\eta \forall f_{i}(\chi^{(i)})\|_{\gamma}^{2} - \chi^{*} \forall f_{i}(\chi^{(i)})^{\dagger}(\chi^{(i)}) + \chi^{*} \|\eta \forall f_{i}(\chi^{(i)})\|_{\gamma}^{2} - \chi^{*} \forall f_{i}(\chi^{(i)})^{\dagger}(\chi^{(i)}) + \chi^{*} \|\eta \forall f_{i}(\chi^{(i)})\|_{\gamma}^{2} = \chi^{*} \forall f_{i}(\chi^{(i)}) + \chi^{*} \|\eta \forall f_{i}(\chi^{(i)})\|_{\gamma}^{2} + \chi^{*} \|\eta \forall f_{i}(\chi^{(i)})\|_$$

Theorem (OGD Regret Bound) After T steps,  $\epsilon = \left[\sum_{i=1}^{T} f_i(\mathbf{x}^{(i)})\right] - \left[\sum_{i=1}^{T} f_i(\mathbf{x}^*)\right] \leq RG\sqrt{T}.$ 

**Claim 1:** For all *i* = 1, ..., *T*,

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

$$\text{Telescoping Sum: } \left( \frac{\|\mathbf{x}^{(i)} - \mathbf{x}^{*}\|_{2}^{2} - \|\mathbf{x}^{(i)} - \mathbf{x}^{*}\|_{2}^{2}}{2\eta} + \left( \frac{\|\mathbf{x}^{(i)} - \mathbf{x}^{*}\|_{2}^{2} - \|\mathbf{x}^{(i)} - \mathbf{x}^{*}\|_{2}^{2}}{2\eta} + \frac{\eta G^{2}}{2\eta} + \frac{$$

Efficient <u>offline</u> optimization method for functions *f* with <u>finite</u> <u>sum structure</u>:

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

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

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

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

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

where  $f_i$  is the loss function for a particular data example  $(\mathbf{a}^{(i)}, \mathbf{y}^{(i)})$ .  $\nabla f_i(\mathbf{x}) = \sum_{i=1}^n \nabla f_i(\mathbf{x})$ 

Example: least squares linear regression.

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

Note that by linearity,  $\nabla f(\mathbf{x}) = \sum_{i=1}^{n} \nabla f_i(\mathbf{x})$ .

**Main idea:** Use random approximate gradient in place of actual gradient.

Pick <u>random</u>  $j \in 1, ..., n$  and update  $\underline{\mathbf{x}}$  using  $\underline{\nabla f_j(\mathbf{x})}$ .  $\mathbb{E} \left[ \nabla f_j(\mathbf{x}) \right] = \frac{1}{n} \nabla f(\mathbf{x}).$ 

$$n\nabla f_j(\mathbf{x})$$
 is an unbiased estimate for the true gradient  $\nabla f(\mathbf{x})$ , but can often be computed in a 1/*n* fraction of the time!

Trade slower convergence for cheaper iterations.

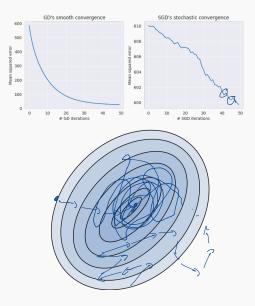
Stochastic first-order oracle for  $f(\mathbf{x}) = \sum_{i=1}^{n} f(\mathbf{x})$ .

- Function Query: For any chosen j,  $\mathbf{x}$ , return  $f_j(\mathbf{x})$
- Gradient Query: For any chosen  $j, \mathbf{x}$ , return  $\nabla f_j(\mathbf{x})$

Stochastic Gradient descent:

- Choose starting vector  $\mathbf{x}^{(1)}$ , learning rate  $\underline{\eta}$
- For i = 1, ..., T:
  - Pick random  $j_i \in 1, \ldots, n$ .
  - $\cdot \mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} \eta \nabla f_{j_i}(\mathbf{x}^{(i)})$
- Return  $\hat{\mathbf{x}} = \frac{1}{T} \sum_{i=1}^{T} \mathbf{x}^{(i)}$

# VISUALIZING SGD



#### 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.
- Lipschitz functions: for all  $\mathbf{x}, j, \|\nabla f_j(\mathbf{x})\|_2 \leq \left(\frac{G'}{n}\right)^2$ 
  - What does this imply about Lipschitz constant of f?
- Starting radius:  $\|\mathbf{x}^* \mathbf{x}^{(1)}\|_2 \le R$ .

### Stochastic Gradient descent:

- Choose  $\mathbf{x}^{(1)}$ , steps *T*, learning rate  $\eta = \frac{D}{G'\sqrt{T}}$ .
- For i = 1, ..., T:
  - Pick random  $j_i \in 1, \ldots, n$ .

• 
$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla f_{j_i}(\mathbf{x}^{(i)})$$

• Return  $\hat{\mathbf{x}} = \frac{1}{T} \sum_{i=1}^{T} \mathbf{x}^{(i)}$ 

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

Only use the fact that step equals gradient in expectation.

#### STOCHASTIC GRADIENT DESCENT ANALYSIS

Claim (SGD Convergence) X = 1 Z X (1) After  $T = \frac{R^2 G'^2}{r^2}$  iterations:  $\mathbb{E}\left[f(\hat{\mathbf{x}}) - f(\mathbf{x}^*)\right] < \epsilon.$  $f\left(\frac{1}{2},\frac{x}{2}\right) \in \frac{1}{2}f(x) + \frac{1}{2}f(y)$ Claim 1:  $f(\hat{\mathbf{x}}) - f(\mathbf{x}^*) \leq \frac{1}{T} \sum_{i=1}^{T} \left[ f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*) \right]$  $= \left( \frac{1}{T} \sum_{i=1}^{T} f(\mathbf{x}^{(i)}) - f(\mathbf{x}^*) \right)$ Prove using Jensen's Inequality:  $f\left(\frac{1}{\tau} \stackrel{\tau}{\lesssim} \chi^{(i)}\right) \leq \frac{1}{\tau} \stackrel{\tau}{\lesssim} f(\chi^{(i)})$ 

#### STOCHASTIC GRADIENT DESCENT ANALYSIS

	Claim (SGD Con	vergence)	ji ~ chif (1,, n)
	After $T = \frac{R^2 G'^2}{\epsilon^2}$ iter	rations: $\mathbb{E}\left[f(\hat{\mathbf{x}}) - f(\mathbf{x}^*)\right] \leq \epsilon.$	f (x ")
	$\mathbb{E}[f(\hat{x}) - f(x^*)]$	$] \leq \frac{1}{T} \sum_{i=1}^{T} \mathbb{E} \left[ f(\mathbf{x}_{\checkmark}^{(i)}) - f(\mathbf{x}^{*}) \right]$	$= \sum_{j=1}^{\infty} f_j(\mathbf{x}^{(i)})$
		$= \frac{1}{T} \sum_{i=1}^{T} \underline{n \mathbb{E}\left[f_{j_i}(\mathbf{x}^{(i)}) - f_{j_i}(\mathbf{x}^*)\right]}$	
offix X	y this (X)	$= \frac{1}{T} \sum_{i=1}^{T} n \mathbb{E} \left( f_{j_i}(\mathbf{x}^{(i)}) - f_{j_i}(\mathbf{x}^{(i)}) \right)$	]
		$\ll \frac{n}{T} \cdot \mathbb{E}\left[\sum_{i=1}^{T} f_{j_i}(\mathbf{x}^{(i)}) - f_{j_i}(\mathbf{x}^{(i)})\right]^{-1}$	= 13.64
		$\leq \frac{n}{T} \cdot \left( R \cdot \frac{G'}{n} \cdot \sqrt{T} \right)$ (by O	GD guarantee.)

#### STOCHASTIC VS. FULL BATCH GRADIENT DESCENT

f(x) = E M(x) Number of iterations for error  $\epsilon$ :  $\| \nabla f(x) \|_{2} = N \cdot \| \nabla h(y) \|_{2}$ • Gradient Descent:  $T \neq \frac{R^2 G^2}{c^2}$ . • Stochastic Gradient Descent:  $T = \left(\frac{R^2 G'^2}{r^2}\right)^2$ Always have  $G \leq G'$ :  $\max_{\mathbf{x}} \|\nabla f(\mathbf{x})\|_{2} \leq \max_{\mathbf{x}} \left( \|\nabla f_{1}(\mathbf{x})\|_{2} + \ldots + \|\nabla f_{n}(\mathbf{x})\|_{2} \right) \leq n \cdot \frac{G'}{n}$ So GD converges strictly faster than SGD. + mox 117f (x) 11 But for a fair comparison: • SGD cost = (# of iterations)  $\cdot O(1)$ + w x 11 fy (x) • GD cost = (# of iterations) · O(n)

We always have  $G \le G'$ . When it is <u>much smaller</u> then GD will perform better. When it is closer to this upper bound, SGD will perform better.

What is an extreme case where G = G'?

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

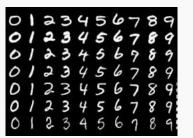
$$\mathbb{E}\left[\|\nabla f_i(\mathbf{x})\|_2^2\right] =$$

$$\mathbb{E}\left[\|\nabla f(\mathbf{x})\|_{2}^{2}\right] = \mathbb{E}\left[\|\sum_{i=1}^{n} \nabla f_{i}(\mathbf{x})\|_{2}^{2}\right] =$$

#### STOCHASTIC VS. FULL BATCH GRADIENT DESCENT

$$|\langle x, x; \rangle - z_i|^2$$
  $a_i$ 

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





#### PRECONDITIONING

**Main idea:** Instead of minimizing  $f(\mathbf{x})$ , find another function  $g(\mathbf{x})$  with the same minimum but which is better suited for first order optimization (e.g., has a smaller conditioner number).

Claim: Let  $h(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}^d$  be an invertible function. Let  $g(\mathbf{x}) = f(h(\mathbf{x}))$ . Then

 $\min_{\mathbf{x}} f(\mathbf{x}) = \min_{\mathbf{x}} g(\mathbf{x}) \quad \text{and} \quad \arg\min_{\mathbf{x}} f(\mathbf{x}) = h\left(\arg\min_{\mathbf{x}} g(\mathbf{x})\right).$ 

First Goal: We need  $g(\mathbf{x})$  to still be convex.

**Claim:** Let **P** be an invertible  $d \times d$  matrix and let  $g(\mathbf{x}) = f(\mathbf{Px})$ .

 $g(\mathbf{x})$  is always convex.

# Second Goal:

# $g(\mathbf{x})$ should have better condition number $\kappa$ than $f(\mathbf{x})$ . Example:

• 
$$f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$$
.  $\kappa_f = \frac{\lambda_1(\mathbf{A}^T\mathbf{A})}{\lambda_d(\mathbf{A}^T\mathbf{A})}$ .  
•  $g(\mathbf{x}) = \|\mathbf{A}\mathbf{P}\mathbf{x} - \mathbf{b}\|_2^2$ .  $\kappa_g = \frac{\lambda_1(\mathbf{P}^T\mathbf{A}^T\mathbf{A}\mathbf{P})}{\lambda_d(\mathbf{P}^T\mathbf{A}^T\mathbf{A}\mathbf{P})}$ 

Third Goal: P should be easy to compute.

Many, many problem specific preconditioners are used in practice. There design is usually a heuristic process.

Example: Diagonal preconditioner.

- · Let  $\mathbf{D} = \operatorname{diag}(\mathbf{A}^T \mathbf{A})$
- Intuitively, we roughly have that  $\mathbf{D} \approx \mathbf{A}^T \mathbf{A}$ .
- · Let  $P=\sqrt{D^{-1}}$

**P** is often called a Jacobi preconditioner. Often works very well in practice!

#### DIAGONAL PRECONDITIONER

-734	1	33	9111	0
-31	-2	108	5946	-19
232	-1	101	3502	10
426	0	-65	12503	9
-373	0	26	9298	0
-236	-2	-94	2398	-1
2024	0	-132	-6904	-25
-2258	-1	92	-6516	6
2229	0	0	11921	-22
338	1	-5	-16118	-23

>> cond(A'*A)	<pre>&gt;&gt; P = sqrt(inv(diag(diag(A'*A)))); &gt;&gt; cond(P*A'*A*P)</pre>
ans =	
	ans =
8.4145e+07	
	10.3878

#### ADAPTIVE STEPSIZES

Another view: If  $g(\mathbf{x}) = f(\mathbf{P}\mathbf{x})$  then  $\nabla g(\mathbf{x}) = \mathbf{P}^T \nabla f(\mathbf{P}\mathbf{x})$ .

 $\nabla g(\mathbf{x}) = \mathbf{P} \nabla f(\mathbf{P} \mathbf{x})$  when **P** is symmetric.

Gradient descent on g:

• For 
$$t = 1, ..., T$$
,  
•  $\mathbf{x}^{(t+1)} = \mathbf{x}^{(t)} - \eta \mathbf{P} \left[ \nabla f(\mathbf{P} \mathbf{x}^{(t)}) \right]$ 

Gradient descent on g:

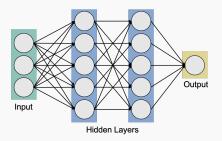
• For 
$$t = 1, ..., T$$
,  
•  $\mathbf{y}^{(t+1)} = \mathbf{y}^{(t)} - \eta \mathbf{P}^2 \left[ \nabla f(\mathbf{y}^{(t)}) \right]$ 

When **P** is diagonal, this is just gradient descent with a different step size for each parameter!

#### ADAPTIVE STEPSIZES

# Algorithms based on this idea:

- AdaGrad
- RMSprop
- Adam optimizer



(Pretty much all of the most widely used optimization methods for training neural networks.)

#### COORDINATE DESCENT

**Main idea:** Trade slower convergence (more iterations) for cheaper iterations.

**Stochastic Gradient Descent:** When  $f(\mathbf{x}) = \sum_{i=1}^{n} f_i(\mathbf{x})$ , approximate  $\nabla f(\mathbf{x})$  with  $\nabla f_i(\mathbf{x})$  for randomly chosen *i*.

**Main idea:** Trade slower convergence (more iterations) for cheaper iterations.

**Stochastic Coordinate Descent:** Only compute a <u>single random</u> <u>entry</u> of  $\nabla f(\mathbf{x})$  on each iteration:

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\mathbf{x}) \\ \frac{\partial f}{\partial x_2}(\mathbf{x}) \\ \vdots \\ \frac{\partial f}{\partial x_d}(\mathbf{x}) \end{bmatrix} \qquad \nabla_i f(\mathbf{x}) = \begin{bmatrix} 0 \\ \frac{\partial f}{\partial x_i}(\mathbf{x}) \\ \vdots \\ 0 \end{bmatrix}$$

Update:  $\mathbf{x}^{(t+1)} \leftarrow \mathbf{x}^{(t)} + \eta \nabla_i f(\mathbf{x}^{(t)})$ .

When **x** has *d* parameters, computing  $\nabla_i f(\mathbf{x})$  often costs just a 1/d fraction of what it costs to compute  $\nabla f(\mathbf{x})$ 

**Example:**  $f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$  for  $\mathbf{A} \in \mathbb{R}^{n \times d}$ ,  $\mathbf{x} \in \mathbb{R}^d$ ,  $\mathbf{b} \in \mathbb{R}^n$ .

$$\cdot \nabla f(\mathbf{x}) = 2\mathbf{A}^{\mathsf{T}}\mathbf{A}\mathbf{x} - 2\mathbf{A}^{\mathsf{T}}\mathbf{b}.$$

• 
$$\nabla_i f(\mathbf{x}) = 2 \left[ \mathbf{A}^T \mathbf{A} \mathbf{x} \right]_i - 2 \left[ \mathbf{A}^T \mathbf{b} \right].$$

# Stochastic Coordinate Descent:

- Choose number of steps T and step size  $\eta$ .
- For i = 1, ..., T:
  - Pick random  $j_i \in 1, \ldots, d$ .

• 
$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \eta \nabla_{j_i} f(\mathbf{x}^{(i)})$$

• Return 
$$\hat{\mathbf{x}} = \frac{1}{T} \sum_{i=1}^{T} \mathbf{x}^{(i)}$$
.

**Theorem (Stochastic Coordinate Descent convergence)** Given a G-Lipschitz function f with minimizer  $\mathbf{x}^*$  and initial point  $\mathbf{x}^{(1)}$  with  $\|\mathbf{x}^{(1)} - \mathbf{x}^*\|_2 \leq R$ , SCD with step size  $\eta = \frac{1}{Rd}$ satisfies the guarantee:

$$\mathbb{E}[f(\hat{\mathbf{x}}) - f(\mathbf{x}^*)] \le \frac{2GR}{\sqrt{T/d}}$$

Often it doesn't make sense to sample *i* uniformly at random:

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -.5 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 & 0 & 0 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 10 \\ 42 \\ -11 \\ -51 \\ 34 \\ -22 \end{bmatrix}$$

Select indices *i* proportional to  $\|\mathbf{a}_i\|_2^2$ :

Pr[select index *i* to update] = 
$$\frac{\|\mathbf{a}_i\|_2^2}{\sum_{j=1}^d \|\mathbf{a}_j\|_2^2} = \frac{\|\mathbf{a}_i\|_2^2}{\|\mathbf{A}\|_2^2}$$