CS-GY 9223 I: Lecture 7
Preconditioning, acceleration, coordinate decent, etc.

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### LOGISTICS

- Self-proctored, 2-hour midterm to be taken anytime next week.
- <u>No Collaboration</u> allowed at all. Or outside resources. Just use your own notes and material from the class.
- Sample problems are available on course website. We can review during office hours tomorrow or next week.
- You should have received an invite to Gradescope.
   Hopefully tonight/tomorrow I can upload a "practice test" to make sure their system works.

### **GRADIENT DESCENT**

## **Conditions:**

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

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

Bounded gradients (Lipschitz function):

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

### **Theorem**

GD Convergence Bound] (Projected) Gradient Descent returns  $\hat{\mathbf{x}}$  with  $f(\hat{\mathbf{x}}) \leq \min_{\mathbf{x} \in \mathcal{S}} f(\mathbf{x}) + \epsilon$  after

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

### ONLINE GRADIENT DESCENT

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

## **Conditions:**

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

# Theorem (OGD Regret Bound)

After T steps, 
$$\left[\sum_{i=1}^{T} f_i(\mathbf{x}^{(i)})\right] - \left[\sum_{i=1}^{T} f_i(\mathbf{x}^*)\right] \leq RG\sqrt{T}$$
. I.e. the average regret  $\frac{1}{T}\left[\sum_{i=1}^{T} f_i(\mathbf{x}^{(i)})\right]$  is  $\leq \epsilon$  after:

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

### STOCHASTIC GRADIENT DESCENT

# **Conditions:**

- Finite sum structure:  $f(\mathbf{x}) = \sum_{i=1}^{n} f_i(\mathbf{x})$ , with  $f_1, \dots, f_n$  all convex.
- Lipschitz functions: for all  $\mathbf{x}$ , j,  $\|\nabla f_j(\mathbf{x})\|_2 \leq \frac{G'}{n}$ .
- Starting radius:  $\|\mathbf{x}^* \mathbf{x}^{(1)}\|_2 \leq R$ .

# Theorem (SGD Regret Bound)

Stochastic Gradient Descent returns  $\hat{\mathbf{x}}$  with

$$\mathbb{E}[f(\hat{\mathbf{x}})] \leq \min_{\mathbf{x} \in \mathcal{S}} f(\mathbf{x}) + \epsilon \text{ after }$$

$$T = \frac{R^2 G'^2}{\epsilon^2}$$
 iterations.

We always have that G' > G, but iterations are typically cheaper by a factor of n.

### BEYOND THE BASIC BOUNDS

Can our convergence bounds be tightened for certain functions? Can they guide us towards faster algorithms?

## Goals:

- Improve  $\epsilon$  dependence below  $1/\epsilon^2$ .
  - Ideally  $1/\epsilon$  or  $\log(1/\epsilon)$ .
- · Reduce or eliminate dependence on G and R.
- Further take advantage of structure in the data (e.g. repetition in features in addition to data points).

### **SMOOTHNESS**

# Definition ( $\beta$ -smoothness)

A function f is  $\beta$  smooth if, for all x, y

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 \le \frac{\beta}{\beta} \|\mathbf{x} - \mathbf{y}\|_2$$

After some calculus (see Lem. 3.4 in **Bubeck's book**), this implies:  $[f(\mathbf{y}) - f(\mathbf{x})] - \nabla f(\mathbf{x})^T (\mathbf{y} - \mathbf{x}) \le \frac{\beta}{2} ||\mathbf{x} - \mathbf{y}||_2^2$ 

For a scalar valued function f, equivalent to  $f''(x) \leq \beta$ .

## **SMOOTHNESS**

Recall from definition of convexity that:

$$f(\mathbf{y}) - f(\mathbf{x}) \ge \nabla f(\mathbf{x})^{\mathsf{T}} (\mathbf{y} - \mathbf{x})$$

So now we have an upper and lower bound.

$$0 \le [f(\mathbf{y}) - f(\mathbf{x})] - \nabla f(\mathbf{x})^{\mathsf{T}}(\mathbf{y} - \mathbf{x}) \le \frac{\beta}{2} \|\mathbf{x} - \mathbf{y}\|_{2}^{2}$$

## **GUARANTEED PROGRESS**

Previously learning rate/step size  $\eta$  depended on G. Now choose it based on  $\beta$ :

$$\mathbf{x}^{(t+1)} \leftarrow \mathbf{x}^{(t)} - \frac{1}{\beta} \nabla f(\mathbf{x}^{(t)})$$

Progress per step of gradient descent:

$$\left[ f(\mathbf{x}^{(t+1)}) - f(\mathbf{x}^{(t)}) \right] - \nabla f(\mathbf{x}^{(t)})^{\mathsf{T}} (\mathbf{x}^{(t+1)} - \mathbf{x}^{(t)}) \le \frac{\beta}{2} \|\mathbf{x}^{(t)} - \mathbf{x}^{(t+1)}\|_{2}^{2}$$

$$\left[ f(\mathbf{x}^{(t+1)}) - f(\mathbf{x}^{(t)}) \right] + \frac{1}{\beta} \|\nabla f(\mathbf{x}^{(t)})\|_2^2 \le \frac{\beta}{2} \|\frac{1}{\beta} \nabla f(\mathbf{x}^{(t)})\|_2^2$$

$$f(\mathbf{x}^{(t)}) - f(\mathbf{x}^{(t+1)}) \ge \frac{1}{2\beta} \|\nabla f(\mathbf{x}^{(t)})\|_2^2$$

# Theorem (GD convergence for $\beta$ -smooth functions.)

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

$$f(\mathbf{x}^{(T)}) - f(\mathbf{x}^*) \le \frac{2\beta R^2}{T - 1}$$

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

### STRONG CONVEXITY

# Definition ( $\alpha$ -strongly convex)

A convex function f is  $\alpha$ -strongly convex if, for all x, y

$$[f(\mathbf{y}) - f(\mathbf{x})] - \nabla f(\mathbf{x})^{\mathsf{T}} (\mathbf{y} - \mathbf{x}) \ge \frac{\alpha}{2} \|\mathbf{x} - \mathbf{y}\|_{2}^{2}$$

 $\alpha$  is a parameter that will depend on our function.

For a twice-differentiable scalar valued function f, equivalent to  $f''(x) \ge \alpha$ .

### **GD FOR STRONGLY CONVEX FUNCTION**

# Gradient descent for strongly convex functions:

- · Choose number of steps T.
- For i = 1, ..., T:

• 
$$\eta = \frac{2}{\alpha \cdot (i+1)}$$

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

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

# Theorem (GD convergence for $\alpha$ -strongly convex functions.)

Let f be an  $\alpha$ -strongly convex function and assume we have that, for all  $\mathbf{x}$ ,  $\|\nabla f(\mathbf{x})\|_2 \leq \mathbf{G}$ . If we run GD for T steps (with adaptive step sizes) we have:

$$f(\hat{\mathbf{x}}) - f(\mathbf{x}^*) \le \frac{2G^2}{\alpha(T-1)}$$

Corollary: If  $T = O\left(\frac{G^2}{\alpha \epsilon}\right)$  we have  $f(\hat{\mathbf{x}}) - f(\mathbf{x}^*) \le \epsilon$ 

What if f is both  $\beta$ -smooth and  $\alpha$ -strongly convex?

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

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

# 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:

$$\|\mathbf{x}^{(T)} - \mathbf{x}^*\|_2^2 \le e^{-(T-1)\frac{\alpha}{\beta}} \|\mathbf{x}^{(1)} - \mathbf{x}^*\|_2^2$$

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

Is it better if  $\kappa$  is large or small?

Converting to more familiar form: Using that fact the  $\nabla f(\mathbf{x}^*) = \mathbf{0}$  along with

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

we have:

$$\|\mathbf{x}^{(1)} - \mathbf{x}^*\|_2^2 \le \frac{2}{\alpha} \left[ f(\mathbf{x}^{(1)}) - f(\mathbf{x}^*) \right]$$
$$\|\mathbf{x}^{(T)} - \mathbf{x}^*\|_2^2 \ge \frac{2}{\beta} \left[ f(\mathbf{x}^{(T)}) - f(\mathbf{x}^*) \right]$$

# Corollary (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:

$$f(\mathbf{x}^{(T)}) - f(\mathbf{x}^*) \le \frac{\beta}{\alpha} e^{-(T-1)\frac{\alpha}{\beta}} \cdot \left[ f(\mathbf{x}^{(1)}) - f(\mathbf{x}^*) \right]$$

Corollary: If  $T = O\left(\frac{\beta}{\alpha}\log(\beta/\alpha\epsilon)\right) = O(\kappa\log(\kappa/\epsilon))$  we have:

$$f(\mathbf{x}^{(T)}) - f(\mathbf{x}^*) \le \epsilon \left[ f(\mathbf{x}^{(1)}) - f(\mathbf{x}^*) \right]$$

Alternative Corollary: If  $T = O\left(\frac{\beta}{\alpha}\log(R\beta/\epsilon)\right)$  we have:

$$f(\mathbf{x}^{(T)}) - f(\mathbf{x}^*) \le \epsilon$$

### THE LINEAR ALGEBRA OF CONDITIONING

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

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

For vector **x**, **y**:

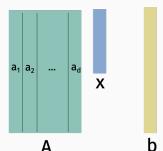
$$\nabla f(\mathbf{x}) - \nabla f(\mathbf{y}) \approx \left[\nabla^2 f(\mathbf{x})\right] (\mathbf{x} - \mathbf{y}).$$

### THE LINEAR ALGEBRA OF CONDITIONING

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

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



#### **HESSIAN MATRICES AND POSITIVE SEMIDEFINITENESS**

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  $\mathbf{y} \in \mathbb{R}^d$ ,  $\mathbf{y}^T \mathbf{H} \mathbf{y} \ge 0$ .

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):

$$H \succeq 0$$
.

We write  $B \succeq A$  or equivalently  $A \succeq B$  to denote that (B - A) is positive semidefinite. This gives a <u>partial ordering</u> on matrices.

#### **HESSIAN MATRICES AND POSITIVE SEMIDEFINITENESS**

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# Definition (Positive Semidefinite (PSD))

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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  $\mathbf{x}$ . Is  $\mathbf{H}$  PSD?

### THE LINEAR ALGEBRA OF CONDITIONING

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

$$\alpha I_{d \times d} \leq H \leq \beta I_{d \times d}$$
,

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:

$$\alpha \leq f''(x) \leq \beta$$
.

### SMOOTH AND STRONGLY CONVEX HESSIAN

$$\alpha I_{d \times d} \leq H \leq \beta I_{d \times d}$$
.

Equivalently for any z,

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

**Exercise:** Show that for  $f(x) = ||Ax - b||_2^2$ ,

$$[f(\mathbf{x}) - f(\mathbf{y})] - \nabla f(\mathbf{x})^{\mathsf{T}} (\mathbf{y} - \mathbf{x}) = (\mathbf{x} - \mathbf{y})^{\mathsf{T}} [2 \mathbf{A}^{\mathsf{T}} \mathbf{A}] (\mathbf{x} - \mathbf{y}).$$

This would imply:

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

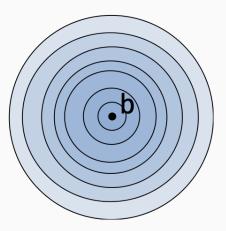
### SIMPLE EXAMPLE

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  $\alpha, \beta$  for this problem?

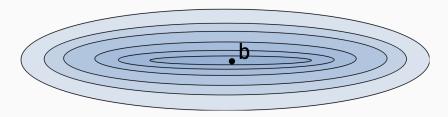
$$\alpha \|\mathbf{z}\|_2^2 \le \mathbf{z}^\mathsf{T} \mathbf{H} \mathbf{z} \le \beta \|\mathbf{z}\|_2^2$$

## **GEOMETRIC VIEW**



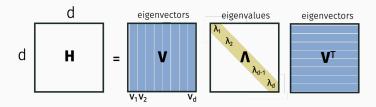
Level sets of  $\|\mathbf{D}\mathbf{x} - \mathbf{b}\|_2^2$  when  $d_1^2 = 1$ ,  $d_2^2 = 1$ .

## **GEOMETRIC VIEW**



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

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

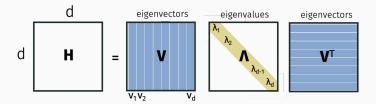


Here **V** is square and orthogonal, so  $\mathbf{V}^T\mathbf{V} = \mathbf{V}\mathbf{V}^T = \mathbf{I}$ . And for each  $\mathbf{v}_i$ , we have:

$$H\mathbf{v}_i = \lambda_i \mathbf{v}_i.$$

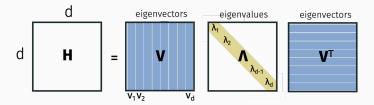
That's what makes  $\mathbf{v}_1, \dots, \mathbf{v}_d$  eigenvectors.

Recall  $VV^T = V^TV = I$ .



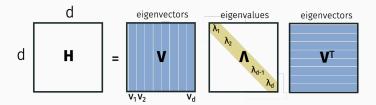
Claim:  $H \Leftrightarrow \lambda_1, ..., \lambda_d \geq 0$ .

Recall  $VV^T = V^TV = I$ .



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

Recall  $VV^T = V^TV = I$ .



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

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

### 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  $\eta = \frac{1}{2\beta}$ ) we have:

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

Goal: Prove for 
$$f(x) = \|Ax - b\|_2^2$$
.

### ALTERNATIVE VIEW OF GRADIENT DESCENT

## Richardson Iteration view:

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

What is the maximum eigenvalue of the symmetric matrix  $\left(\mathbf{I} - \frac{1}{\lambda_{\text{max}}} \mathbf{A}^T \mathbf{A}\right)$  in terms of the eigenvalues  $\lambda_{\text{max}} = \lambda_1 \geq \ldots \geq \lambda_d = \lambda_{\text{min}}$  of  $\mathbf{A}^T \mathbf{A}$ ?

## UNROLLED GRADIENT DESCENT

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

What is the maximum eigenvalue of the symmetric matrix  $\left(\mathbf{I}-\frac{1}{\lambda_{\max}}\mathbf{A}^T\mathbf{A}\right)^T$ ?

So we have  $\|\mathbf{x}^{(T)} - \mathbf{x}^*\|_2 \le$ 

### IMPROVING GRADIENT DESCENT

We now have a <u>really good</u> understanding of gradient descent.

# Number of iterations for $\epsilon$ error:

	G-Lipschitz	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	$O\left(\frac{G^2}{\alpha\epsilon}\right)$	$O\left(\frac{\beta}{\alpha}\log(1/\epsilon)\right)$

How do we use this understanding to design faster algorithms?



#### ACCELERATED GRADIENT DESCENT

# Nesterov's accelerated gradient descent:

$$\begin{aligned} \cdot \ & \mathbf{x}^{(1)} = \mathbf{y}^{(1)} = \mathbf{z}^{(1)} \\ \cdot \ & \text{For } t = 1, \dots, T \\ \cdot \ & \mathbf{y}^{(t+1)} = \mathbf{x}^{(t)} - \frac{1}{\beta} \nabla f(\mathbf{x}^{(t)}) \\ \cdot \ & \mathbf{x}^{(t+1)} = \left(1 + \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right) \mathbf{y}^{(t+1)} + \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \left(\mathbf{y}^{(t+1)} - \mathbf{y}^{(t)}\right) \end{aligned}$$

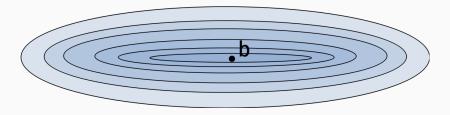
# Theorem (AGD for $\beta$ -smooth, $\alpha$ -strongly convex.)

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?



#### **PRECONDITIONING**

Main idea: Instead of minimizing f(x), find another function g(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 <u>invertible function</u>. Let  $g(\mathbf{x}) = f(h(\mathbf{x}))$ . Then

$$\min_{\mathbf{x}} f(\mathbf{x}) = \min_{\mathbf{x}} g(\mathbf{x})$$
 and  $\underset{\mathbf{x}}{\operatorname{arg min}} f(\mathbf{x}) = h\left(\underset{\mathbf{x}}{\operatorname{arg min}} g(\mathbf{x})\right)$ .

### **PRECONDITIONING**

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

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

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

### **PRECONDITIONING**

## Second Goal:

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

# Example:

$$f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_{2}^{2}. \ \kappa_{f} = \frac{\lambda_{1}(\mathbf{A}^{\mathsf{T}}\mathbf{A})}{\lambda_{d}(\mathbf{A}^{\mathsf{T}}\mathbf{A})}.$$

$$f(\mathbf{x}) = \|\mathbf{A}\mathbf{P}\mathbf{x} - \mathbf{b}\|_{2}^{2}. \ \kappa_{g} = \frac{\lambda_{1}(\mathbf{P}^{\mathsf{T}}\mathbf{A}^{\mathsf{T}}\mathbf{A}\mathbf{P})}{\lambda_{d}(\mathbf{P}^{\mathsf{T}}\mathbf{A}^{\mathsf{T}}\mathbf{A}\mathbf{P})}.$$

**Ideal preconditioner:** Choose P so that  $P^TA^TAP = I$ . For example, could set  $P = \sqrt{(A^TA)^{-1}}$ .

What's the problem with this choice?

### DIAGONAL PRECONDITIONER

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

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

## DIAGONAL PRECONDITIONER

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

### **ADAPTIVE STEPSIZES**

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

 $\nabla g(\mathbf{x}) = \mathbf{P} \nabla f(\mathbf{P}\mathbf{x})$  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:

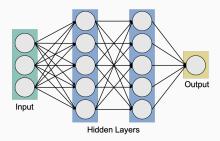
• For 
$$t = 1, ..., T$$
,  
•  $\mathbf{y}^{(t+1)} = \mathbf{y}^{(t)} - \eta \mathbf{P}^2 \left[ \nabla f(\mathbf{y}^{(t)}) \right]$ 

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.)



### STOCHASTIC METHODS

**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.

## STOCHASTIC METHODS

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

Stochastic Coordinate Descent: Only compute a <u>single random</u> entry 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:  $\mathbf{x}^{(t+1)} \leftarrow \mathbf{x}^{(t)} + \eta \nabla_i f(\mathbf{x}^{(t)})$ .

### COORDINATE DESCENT

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

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

### STOCHASTIC COORDINATE DESCENT

## **Stochastic Coordinate Descent:**

- Choose number of steps T and step size  $\eta$ .
- For i = 1, ..., T:
  - Pick random  $j_i \in 1, ..., d$ .
  - $\cdot \mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} \eta \nabla_{j_i} f(\mathbf{x}^{(i)})$
- Return  $\hat{\mathbf{x}} = \frac{1}{T} \sum_{i=1}^{T} \mathbf{x}^{(i)}$ .

## COORDINATE DESCENT

# Theorem (Stochastic Coordinate Descent convergence)

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

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

### IMPORTANCE SAMPLING

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

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

$$\mathbf{b} = \begin{vmatrix} 10 \\ 42 \\ -11 \\ -51 \\ 34 \\ -22 \end{vmatrix}$$

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

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