

UVA CS 6316/4501

– Fall 2016

Machine Learning

Lecture 4: More optimization for Linear Regression

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Where are we? →

Five major sections of this course

- Regression (supervised)
- Classification (supervised)
- Unsupervised models
- Learning theory
- Graphical models

Today →

Regression (supervised)

- Four ways to train / perform optimization for linear regression models
 - Normal Equation
 - Gradient Descent (GD)
 - Stochastic GD
 - Newton's method

- Supervised regression models
 - Linear regression (LR)
 - LR with non-linear basis functions
 - Locally weighted LR
 - LR with Regularizations

Today

- ❑ A Practical Application of Regression Model
- ❑ More ways to train / perform optimization for linear regression models
 - ❑ Gradient
 - ❑ Gradient Descent (GD) for LR
 - ❑ Stochastic GD (SGD)
 - ❑ Newton's method

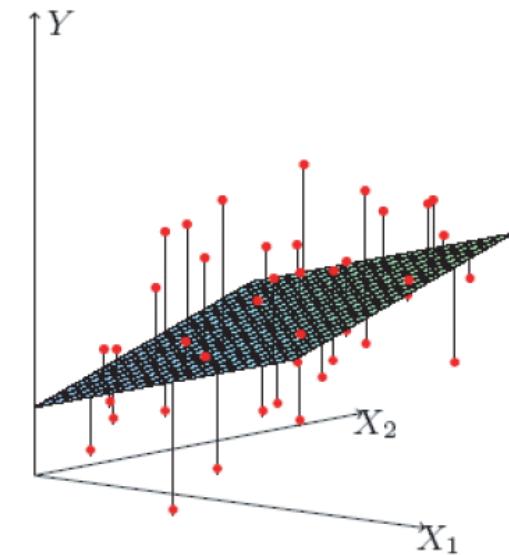
Linear Regression Models

$$[f]: X \rightarrow Y$$

→ e.g. Linear Regression Models

$$\hat{y} = f(x) = \theta_0 + \theta_1 x^1 + \theta_2 x^2$$

- Features:
Living area, distance to campus, # bedroom ...
- Target y:
Rent → Continuous



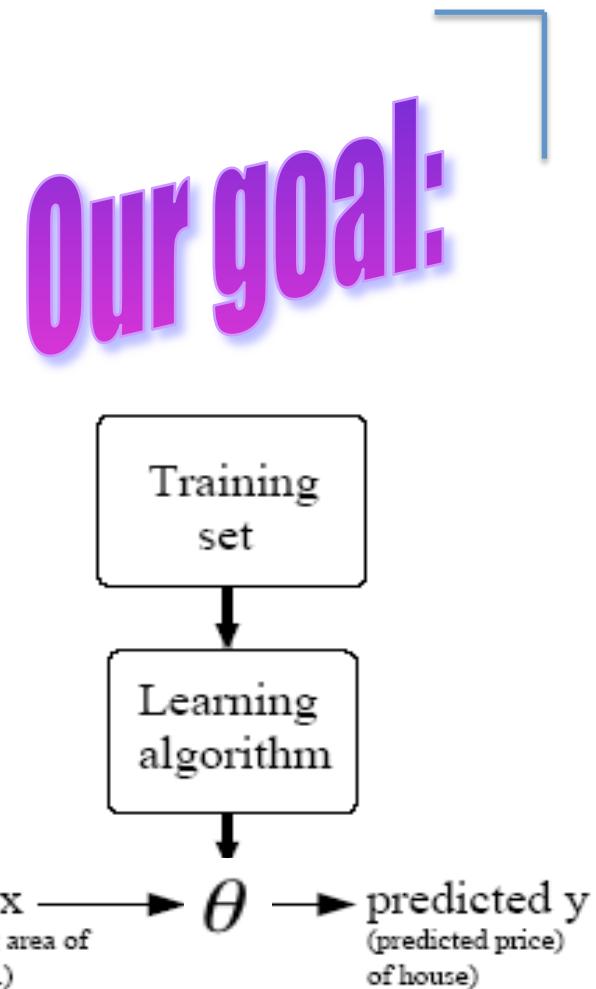
training / learning goal

- Using matrix form, we get the following general representation of the linear function on train set:

$$\hat{Y} = X\theta$$

- Our goal is to pick the optimal θ that minimize the following cost (SSE) function:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^n (\hat{y}_i(\bar{x}_i) - y_i)^2$$



Method I: normal equations

- Write the cost function in matrix form:

$$\begin{aligned}
 J(\theta) &= \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i^T \theta - y_i)^2 \\
 &= \frac{1}{2} (\mathbf{X}\theta - \bar{\mathbf{y}})^T (\mathbf{X}\theta - \bar{\mathbf{y}}) \\
 &= \frac{1}{2} (\theta^T \mathbf{X}^T \mathbf{X}\theta - \theta^T \mathbf{X}^T \bar{\mathbf{y}} - \bar{\mathbf{y}}^T \mathbf{X}\theta + \bar{\mathbf{y}}^T \bar{\mathbf{y}})
 \end{aligned}$$

$$\mathbf{X} = \begin{bmatrix} \cdots & \mathbf{x}_1^T & \cdots \\ \cdots & \mathbf{x}_2^T & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & \mathbf{x}_n^T & \cdots \end{bmatrix} \quad \mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

To minimize $J(\theta)$, take its gradient and set to zero:

$$\Rightarrow \boxed{X^T X\theta = X^T \bar{y}}$$

The normal equations

$$\theta^* = (X^T X)^{-1} X^T \bar{y}$$

$X^T X$ Gram matrix
 \downarrow
 PSD
 \downarrow
 $J(\theta)$ convex
 \downarrow
 $\nabla J(\theta) = 0 \Rightarrow \theta^*$

e.g. A Practical Application of Regression Model

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Movie Reviews and Revenues: An Experiment in Text Regression*

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Abstract

We consider the problem of predicting a movie's opening weekend revenue. Previous work on this problem has used metadata about a movie—e.g., its genre, MPAA rating, and cast—with very limited work making use of text *about* the movie. In this paper, we use the text of film critics' reviews from several sources to predict opening weekend revenue. We describe a new dataset pairing movie reviews with metadata and revenue data, and show that review text can substitute for metadata, and even improve over it, for prediction.

Proceedings of
HLT '2010
Human
Language
Technologies:

I. The Story in Short

- ❖ Use metadata and critics' reviews to predict opening weekend revenues of movies
- ❖ Feature analysis shows what aspects of reviews predict box office success

II. Data

- ❖ 1718 Movies, released 2005-2009
- ❖ Metadata (genre, rating, running time, actors, director, etc.): www.metacritic.com
- ❖ Critics' reviews (~7K): Austin Chronicle, Boston Globe, Entertainment Weekly, LA Times, NY Times, Variety, Village Voice
- ❖ Opening weekend revenues and number of opening screens: www.the-numbers.com

Movie Reviews and Revenues: An Experiment in Text Regression,
Proceedings of HLT '10 Human Language Technologies:

III. Model

- ❖ Linear regression with the elastic net (Zou and Hastie, 2005)

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}=(\beta_0, \boldsymbol{\beta})}{\operatorname{argmin}} \frac{1}{2n} \left[\sum_{i=1}^n \left(y_i - (\beta_0 + \mathbf{x}_i^\top \boldsymbol{\beta}) \right)^2 + \lambda P(\boldsymbol{\beta}) \right]$$

$$P(\boldsymbol{\beta}) = \sum_{j=1}^p \left(\frac{1}{2}(1-\alpha)\beta_j^2 + \alpha|\beta_j| \right)$$

Use linear regression to directly predict the opening weekend gross earnings, denoted y , based on features x extracted from the movie metadata and/or the text of the reviews.

Movie Reviews and Revenues: An Experiment in Text Regression,
Proceedings of HLT '10 Human Language Technologies:

e.g. counts
of a ngram in
the text

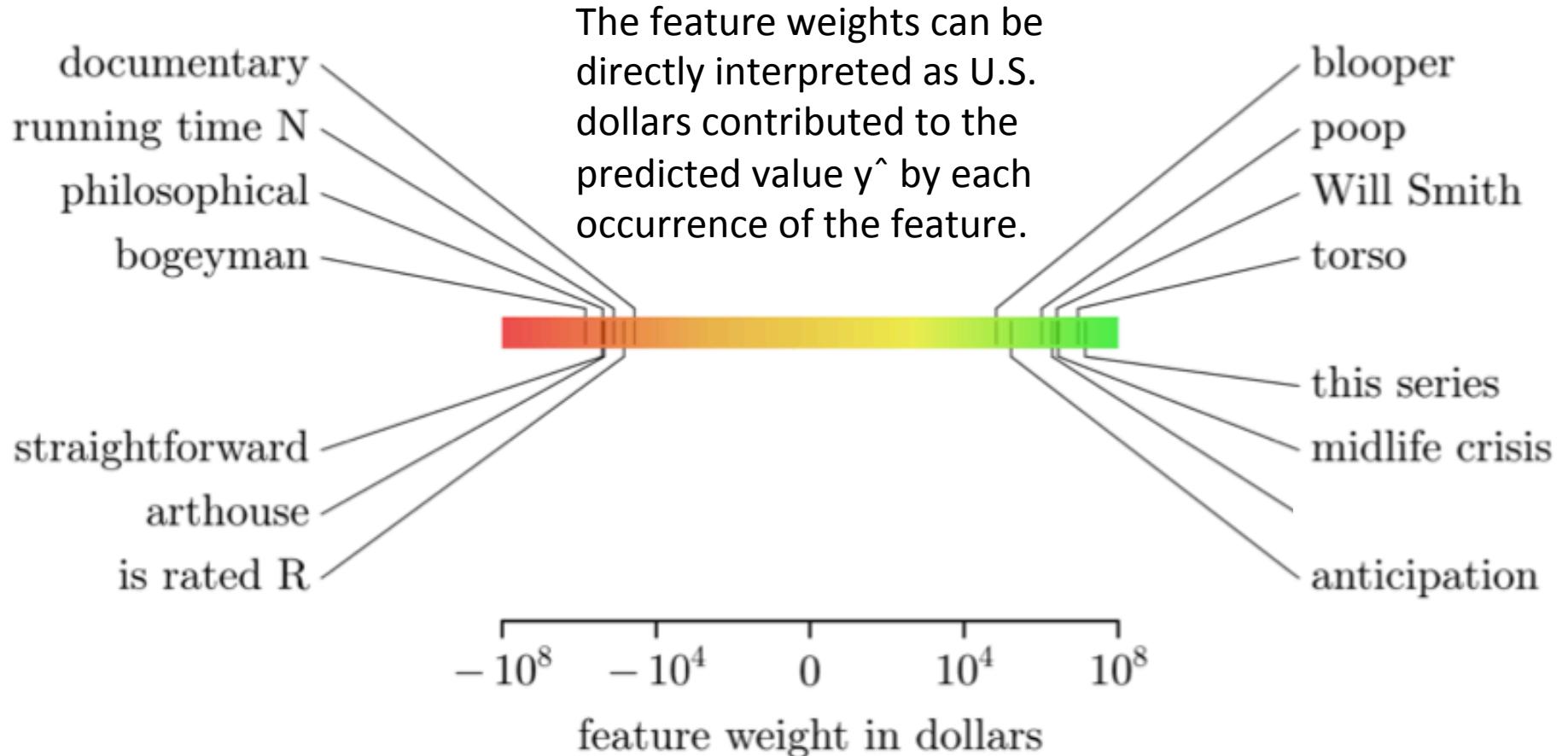
IV. Features

| | |
|------|--|
| I | Lexical n-grams (1,2,3) |
| II | Part-of-speech n-grams (1,2,3) |
| III | Dependency relations (nsubj,advmod,...) |
| Meta | U.S. origin, running time, budget (log), # of opening screens, genre, MPAA rating, holiday release (summer, Christmas, Memorial day,...), star power (Oscar winners, high-grossing actors) |

VIII. Get the Data!

www.ark.cs.cmu.edu/movies-data

V. What May Have Brought You to movies



Today

- ❑ A Practical Application of Regression Model
- ❑ More ways to train / perform optimization for linear regression models
 - ❑ Gradient Descent
 - ❑ Gradient Descent (GD) for LR
 - ❑ Stochastic GD (SGD)
 - ❑ Newton's method

Review: Definitions of gradient

(from review handout)

Suppose that $f : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ is a function that takes as input a matrix A of size $m \times n$ and returns a real value. Then the **gradient** of f (with respect to $A \in \mathbb{R}^{m \times n}$) is the matrix of

→ Denominator layout

$$\nabla_A f(A) \in \mathbb{R}^{m \times n} = \begin{bmatrix} \frac{\partial f(A)}{\partial A_{11}} & \frac{\partial f(A)}{\partial A_{12}} & \dots & \frac{\partial f(A)}{\partial A_{1n}} \\ \frac{\partial f(A)}{\partial A_{21}} & \frac{\partial f(A)}{\partial A_{22}} & \dots & \frac{\partial f(A)}{\partial A_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(A)}{\partial A_{m1}} & \frac{\partial f(A)}{\partial A_{m2}} & \dots & \frac{\partial f(A)}{\partial A_{mn}} \end{bmatrix}$$

Review: Definitions of gradient

(from http://en.wikipedia.org/wiki/Matrix_calculus#Scalar-by-matrix)

The derivative of a scalar y function of a matrix \mathbf{X} of independent variables, with respect to the matrix $\mathbf{X}_{p \times q}$, is given as

→ Numerator layout

$$\frac{\partial y}{\partial \mathbf{X}} = \begin{bmatrix} \frac{\partial y}{\partial x_{11}} & \frac{\partial y}{\partial x_{21}} & \cdots & \frac{\partial y}{\partial x_{p1}} \\ \frac{\partial y}{\partial x_{12}} & \frac{\partial y}{\partial x_{22}} & \cdots & \frac{\partial y}{\partial x_{p2}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y}{\partial x_{1q}} & \frac{\partial y}{\partial x_{2q}} & \cdots & \frac{\partial y}{\partial x_{pq}} \end{bmatrix}$$

Notice that the indexing of the gradient with respect to \mathbf{X} is transposed as compared with the indexing of \mathbf{X} .

→ numerator layout

Review: Definitions of gradient (from review handout)

- Size of gradient is always the same as the size of

→ Denominator layout

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix} \in \mathbb{R}^n \quad \text{if } x \in \mathbb{R}^n$$

(from http://en.wikipedia.org/wiki/Matrix_calculus#Scalar-by-vector)

The derivative of a scalar y by a vector $\mathbf{x} =$

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \text{ is}$$

→ Numerator layout

$$\frac{\partial y}{\partial \mathbf{x}} = \left[\frac{\partial y}{\partial x_1} \quad \frac{\partial y}{\partial x_2} \quad \cdots \quad \frac{\partial y}{\partial x_n} \right]$$

This gradient is a $1 \times n$ row vector whose entries respectively contain the n partial derivatives

→ numerator layout

A little bit more about [Optimization]

- Objective function $F(x) \rightarrow J(\theta)$
- Variables x $\rightarrow \theta$
- Constraints $\rightarrow \theta \in \mathbb{R}^P$

To find values of the variables
that minimize or maximize the objective function
while satisfying the constraints

e.g. Gradient Descent (Steepest Descent)

A first-order optimization algorithm.

To find a local minimum of a function using gradient descent, one takes steps proportional to the negative of the gradient of the function at the current point.

The gradient points in the direction of the greatest rate of increase of the function and its magnitude is the slope of the graph in that direction

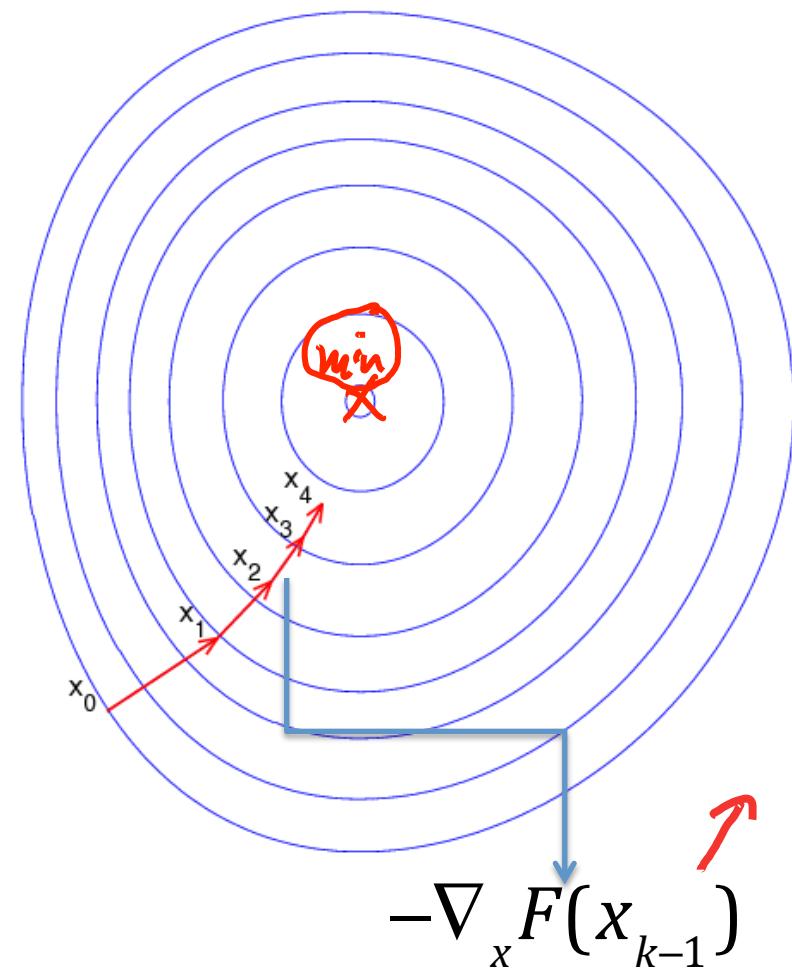
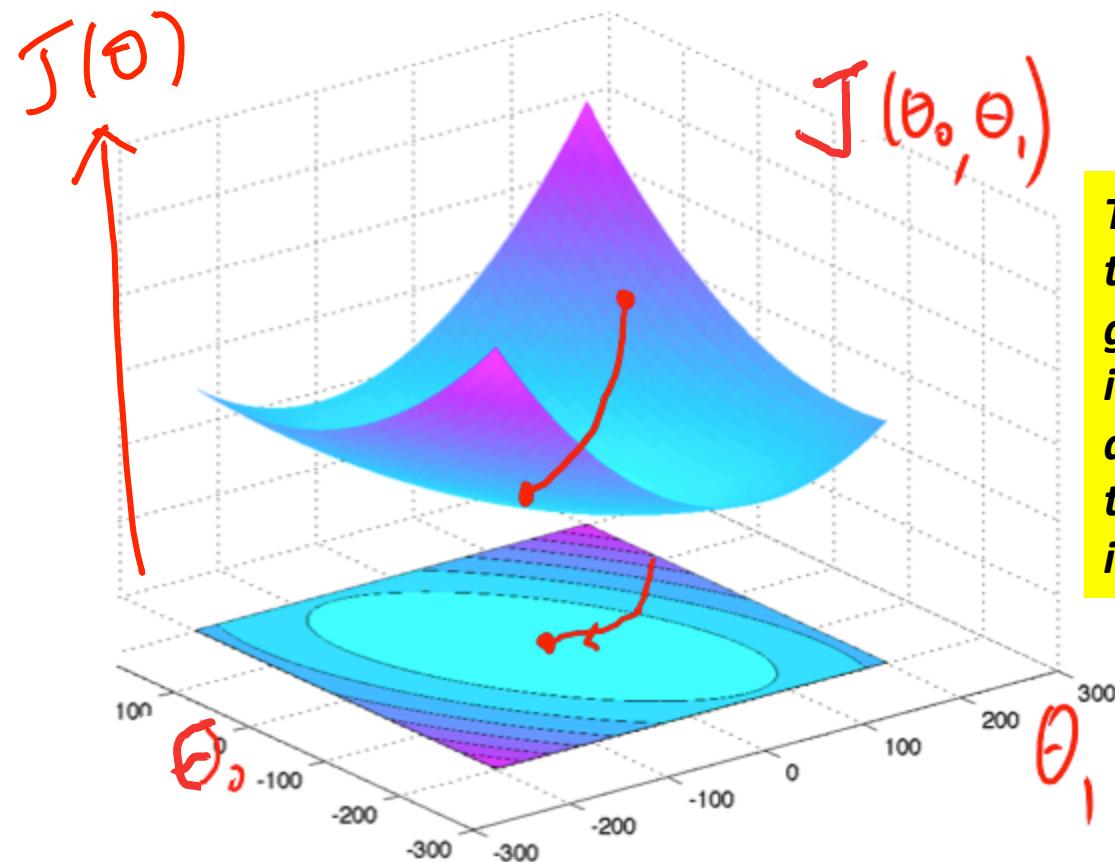


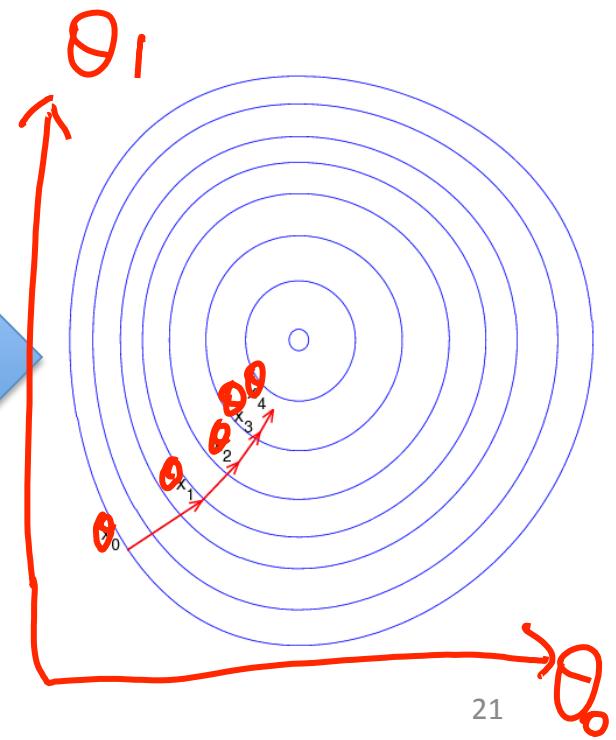
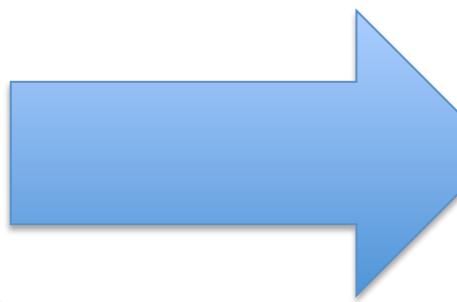
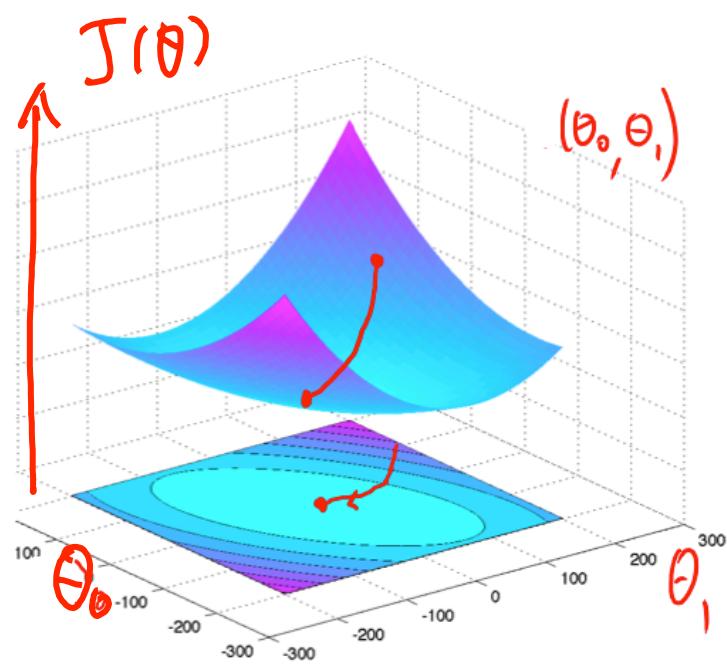
Illustration of Gradient Descent (2D case)



The gradient points in the direction of the greatest rate of increase of the function and its magnitude is the slope of the graph in that direction



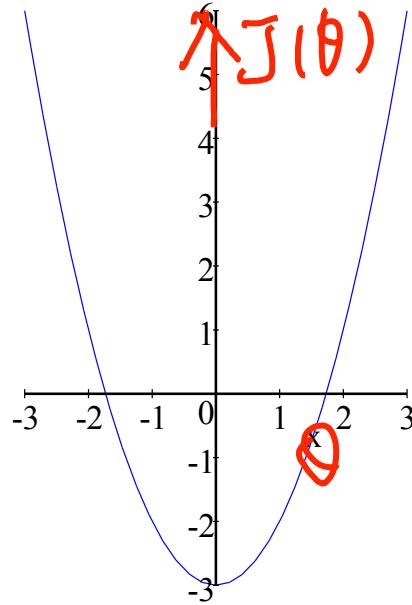
Dr. Yanj



Gradient Descent (GD)

- Initialize $k=0$, choose x_0
- While $k < k_{\max}$ For the k -th epoch

$$x_k = x_{k-1} - \alpha \nabla_x F(x_{k-1})$$

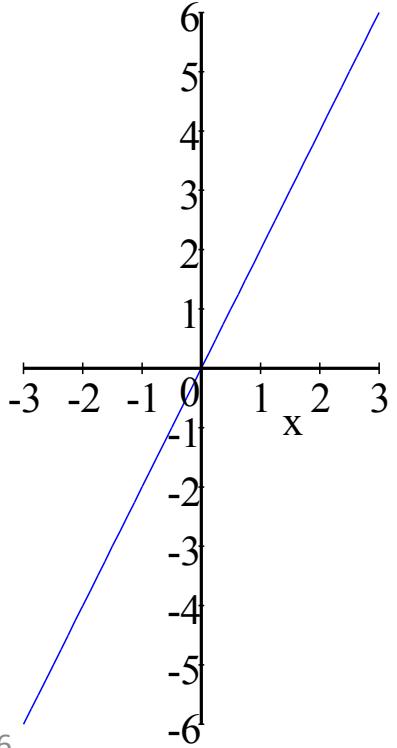


Review: Derivative of a Quadratic Function

$$y = x^2 - 3$$

$$y' = \lim_{h \rightarrow 0} \frac{(x+h)^2 - 3 - (x^2 - 3)}{h}$$

$$y' = \lim_{h \rightarrow 0} \frac{x^2 + 2xh + h^2 - x^2}{h}$$



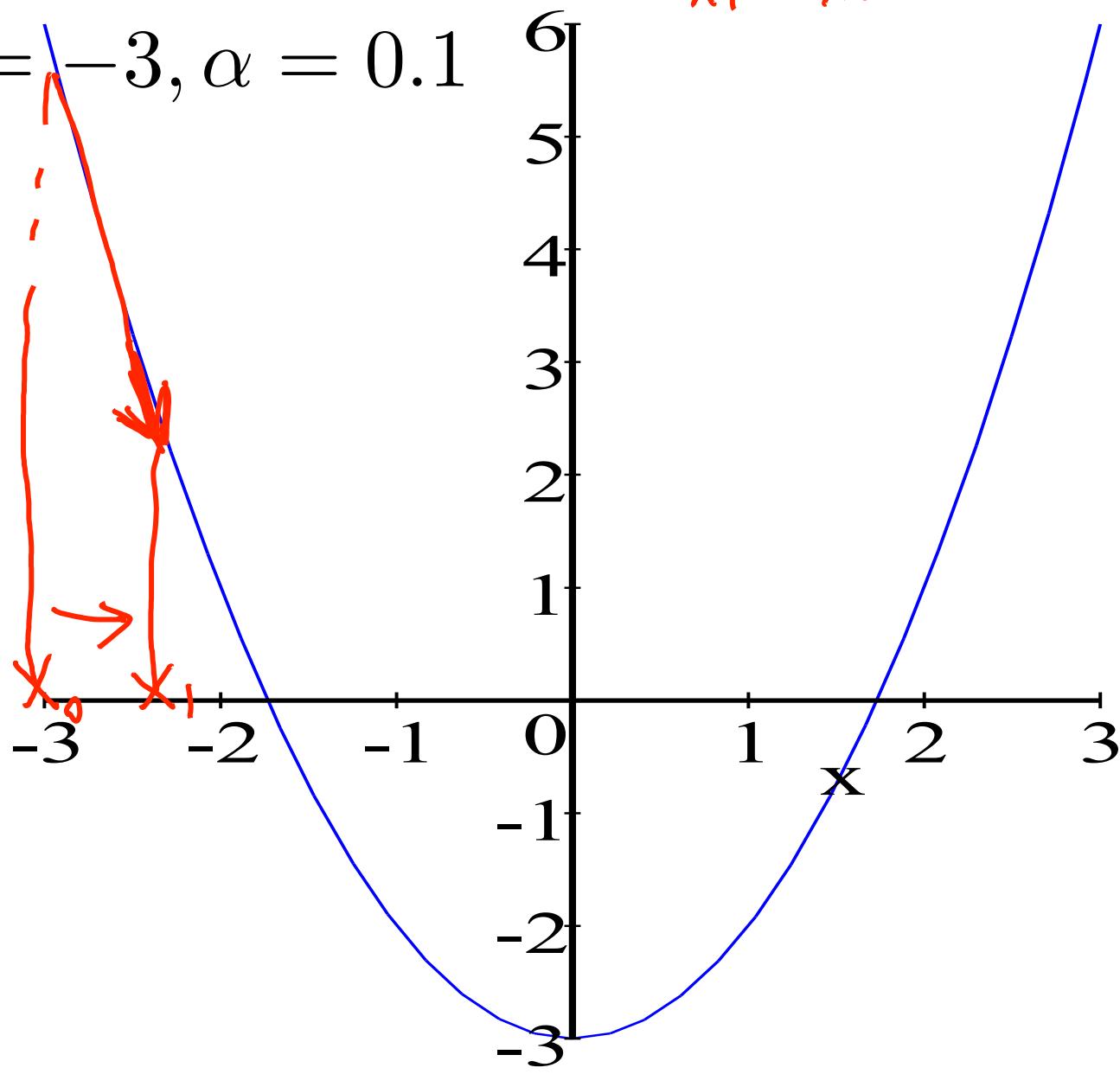
$$y' = \lim_{h \rightarrow 0} 2x + h$$

$$y' = 2x$$

$$y'' = 2$$

$$x_k = x_{k-1} - \alpha \nabla_x F(x_{k-1})$$

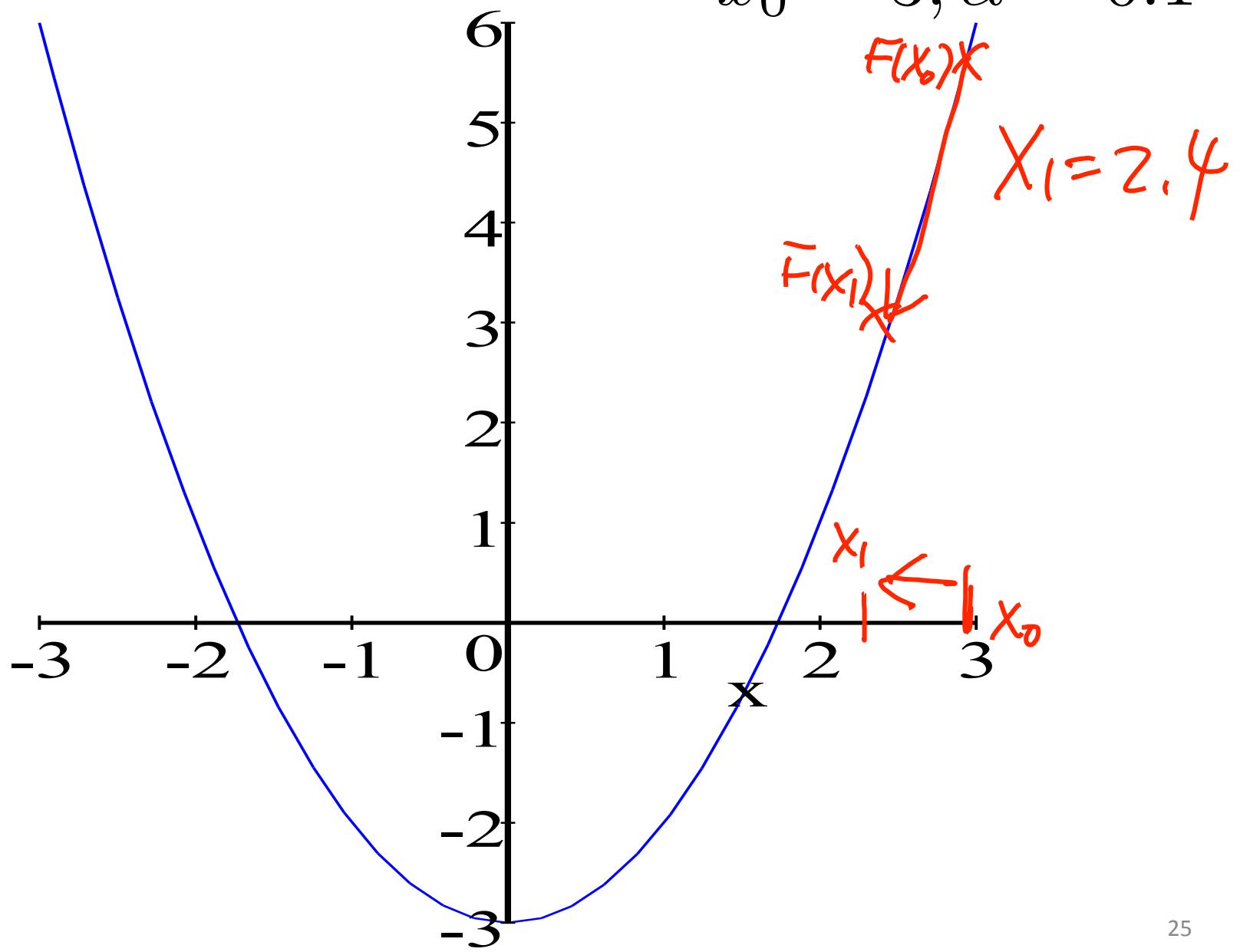
$$x_0 = -3, \alpha = 0.1$$



$$\begin{aligned} X_1 &= X_0 - \alpha \nabla F(X_0) \\ &= -3 \\ &- 2 \times 0.1 \times (-3) \\ &= -2.4 \end{aligned}$$

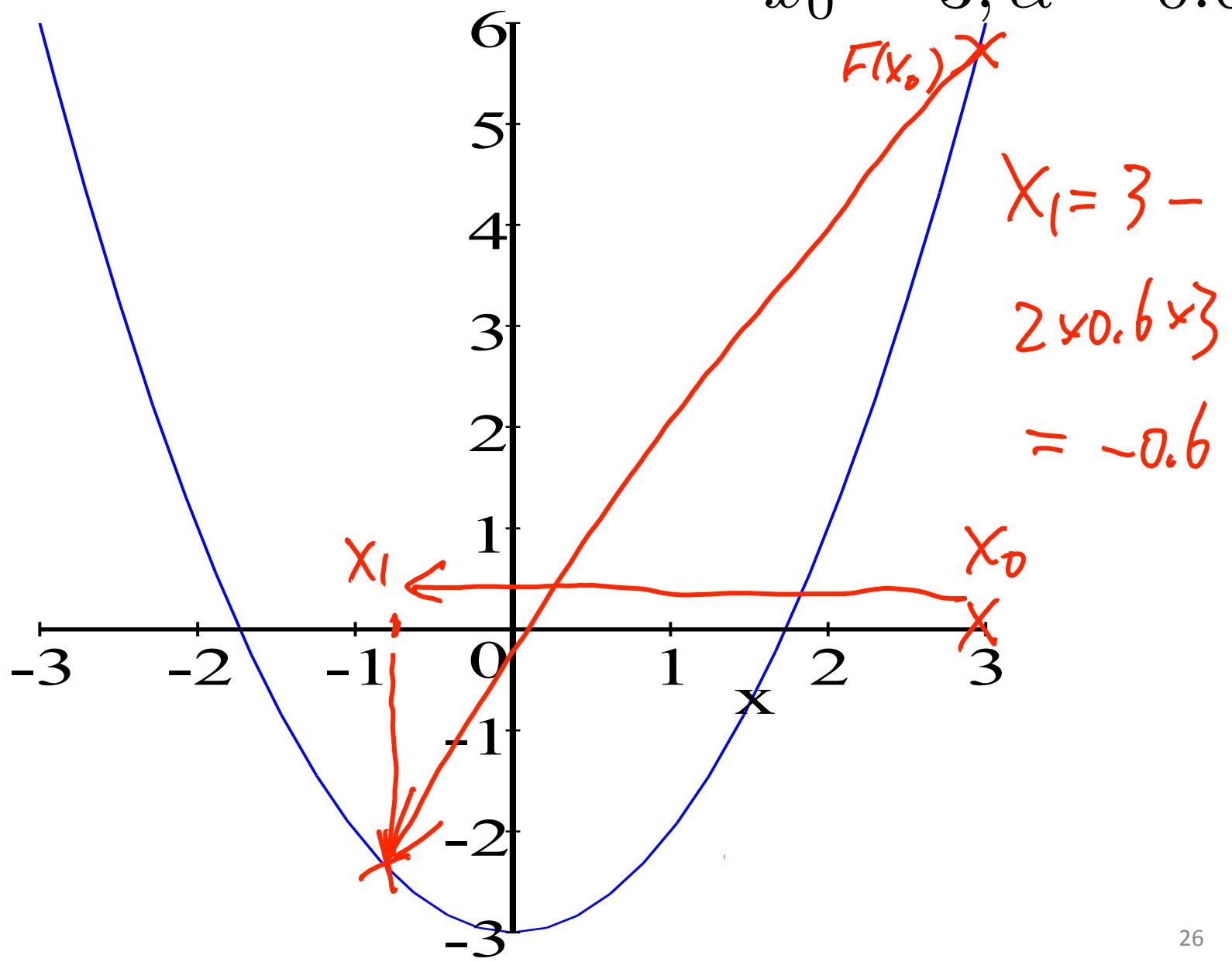
$$x_k = x_{k-1} - \alpha \nabla_x F(x_{k-1})$$

$$x_0 = 3, \alpha = 0.1$$



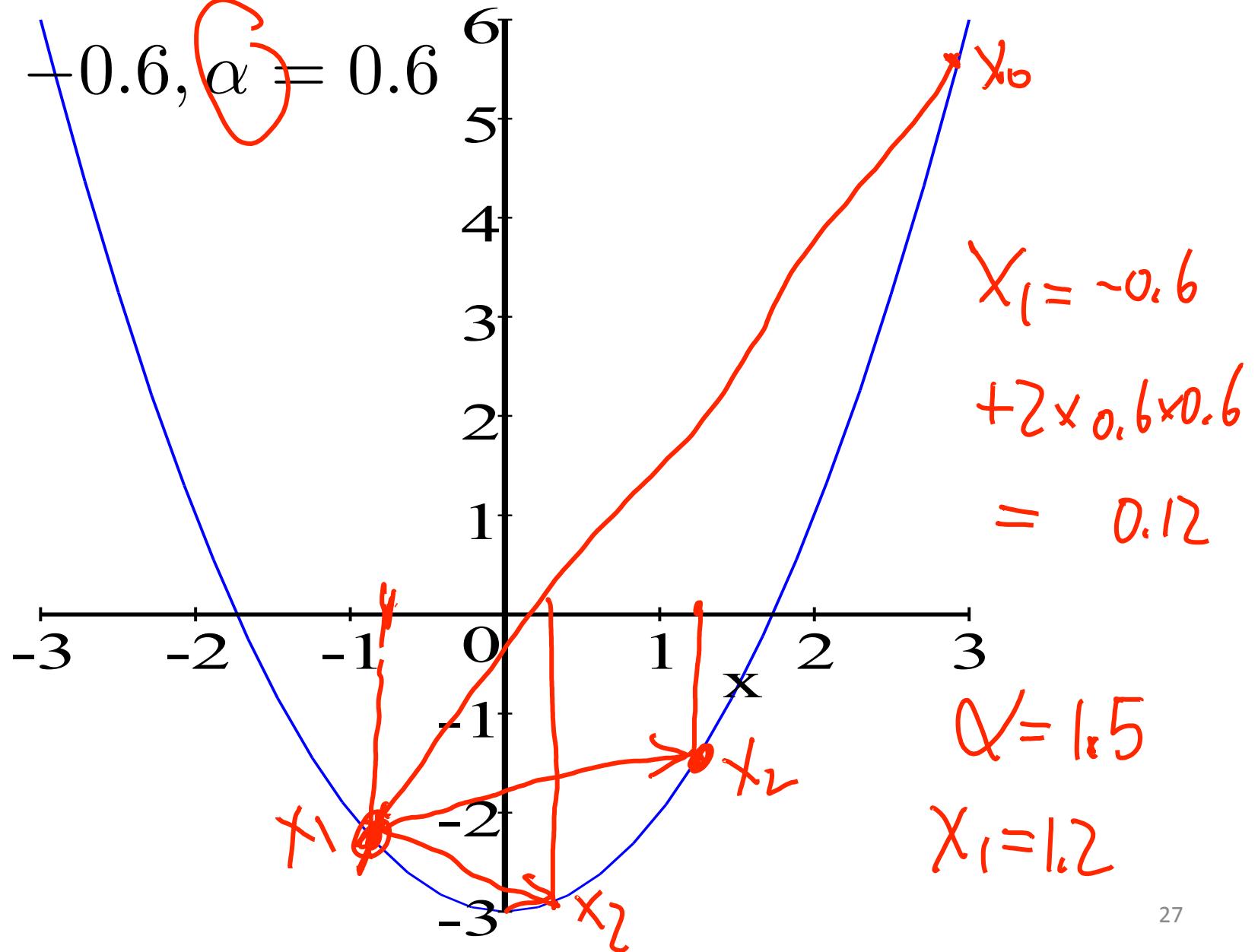
$$x_k = x_{k-1} - \alpha \nabla_x F(x_{k-1})$$

$$x_0 = 3, \alpha = 0.6$$

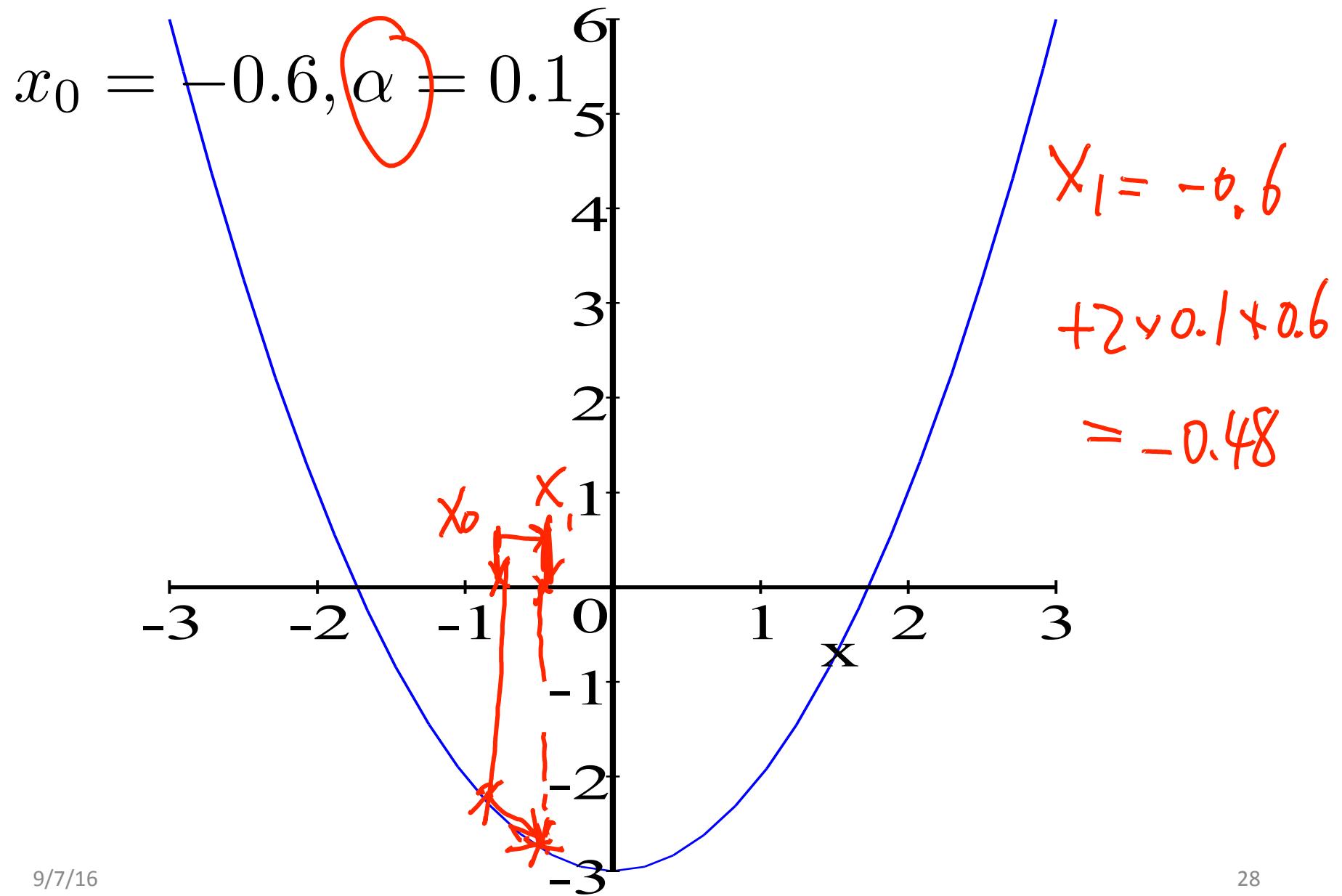


$$x_k = x_{k-1} - \alpha \nabla_x F(x_{k-1})$$

$$x_0 = -0.6, \alpha = 0.6$$



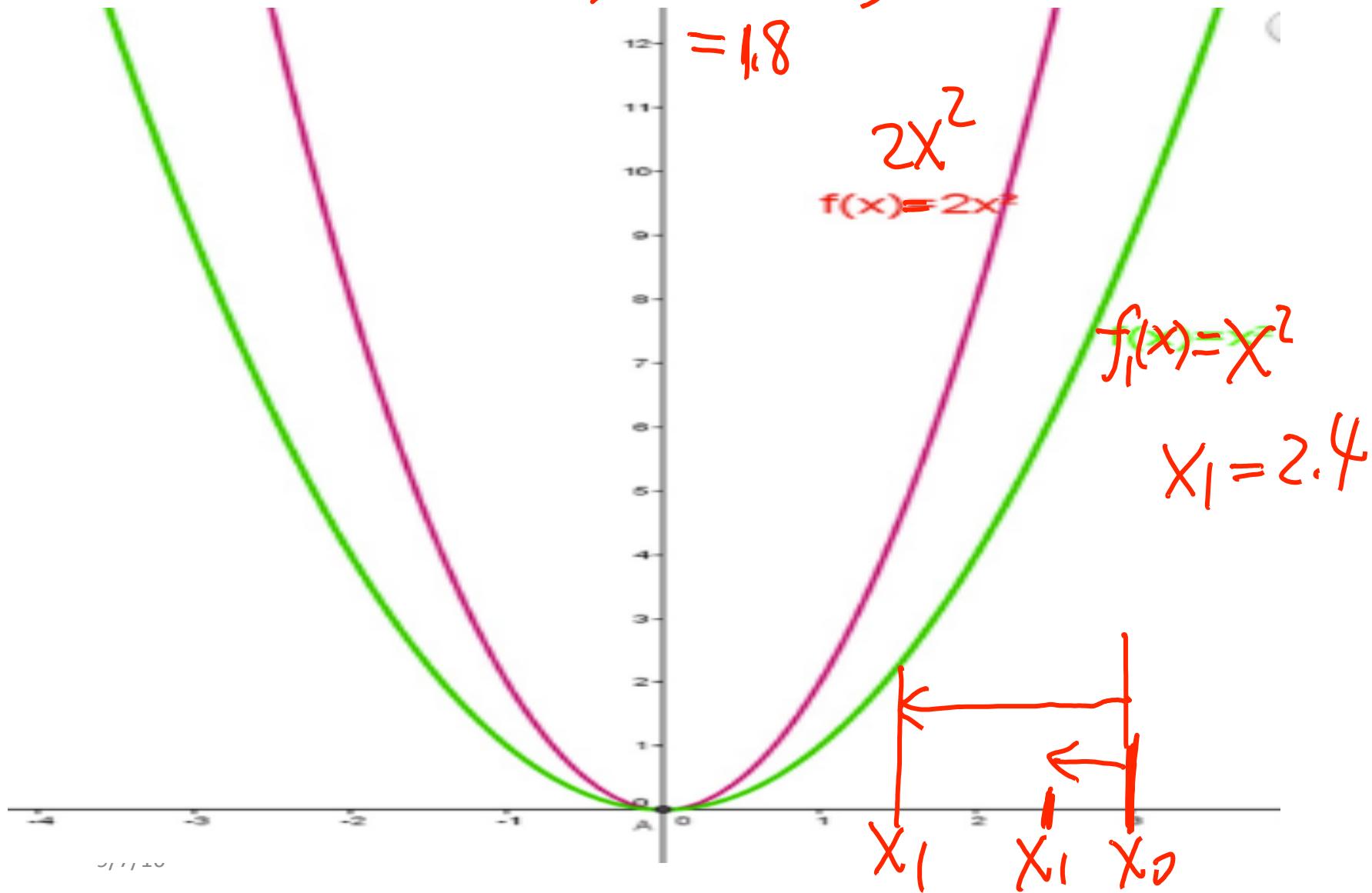
$$x_k = x_{k-1} - \alpha \nabla_x F(x_{k-1})$$

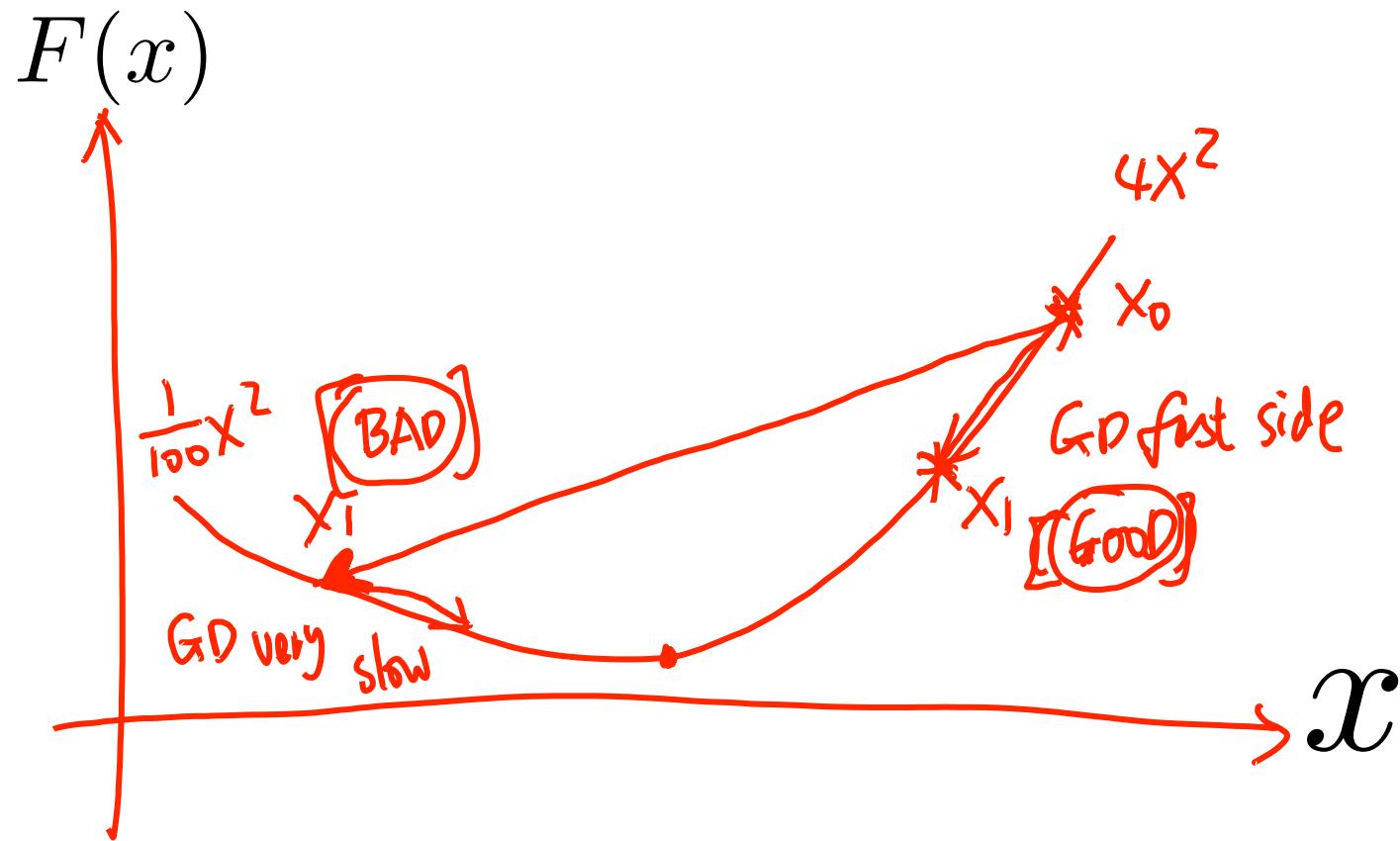


$$x_k = x_{k-1} - \alpha \nabla_x F(x_{k-1})$$

$$x_0 = 3, \alpha = 0.1$$

$$\begin{aligned} x_1 &= 3 - 4 \times 0.1 \times 3 \\ &= 1.8 \end{aligned}$$





Review: Derivative of a Quadratic Function

$$y = x^2 - 3$$

$$y' = \lim_{h \rightarrow 0} \frac{(x+h)^2 - 3 - (x^2 - 3)}{h}$$

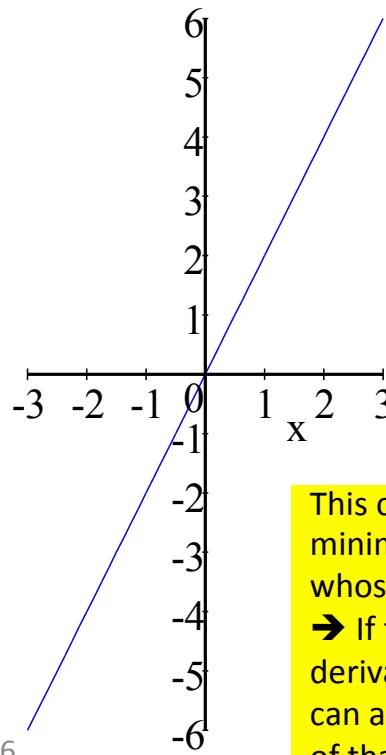
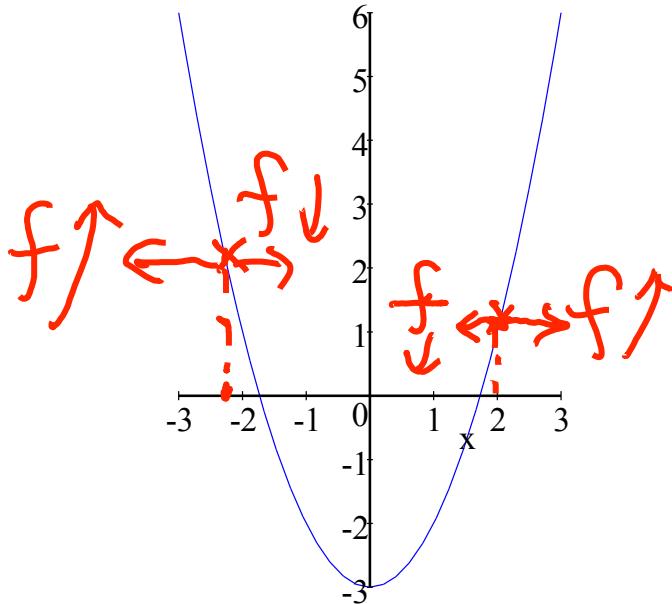
$$y' = \lim_{h \rightarrow 0} \frac{x^2 + 2xh + h^2 - x^2}{h}$$

$$y' = \lim_{h \rightarrow 0} 2x + h$$

$$y' = 2x$$

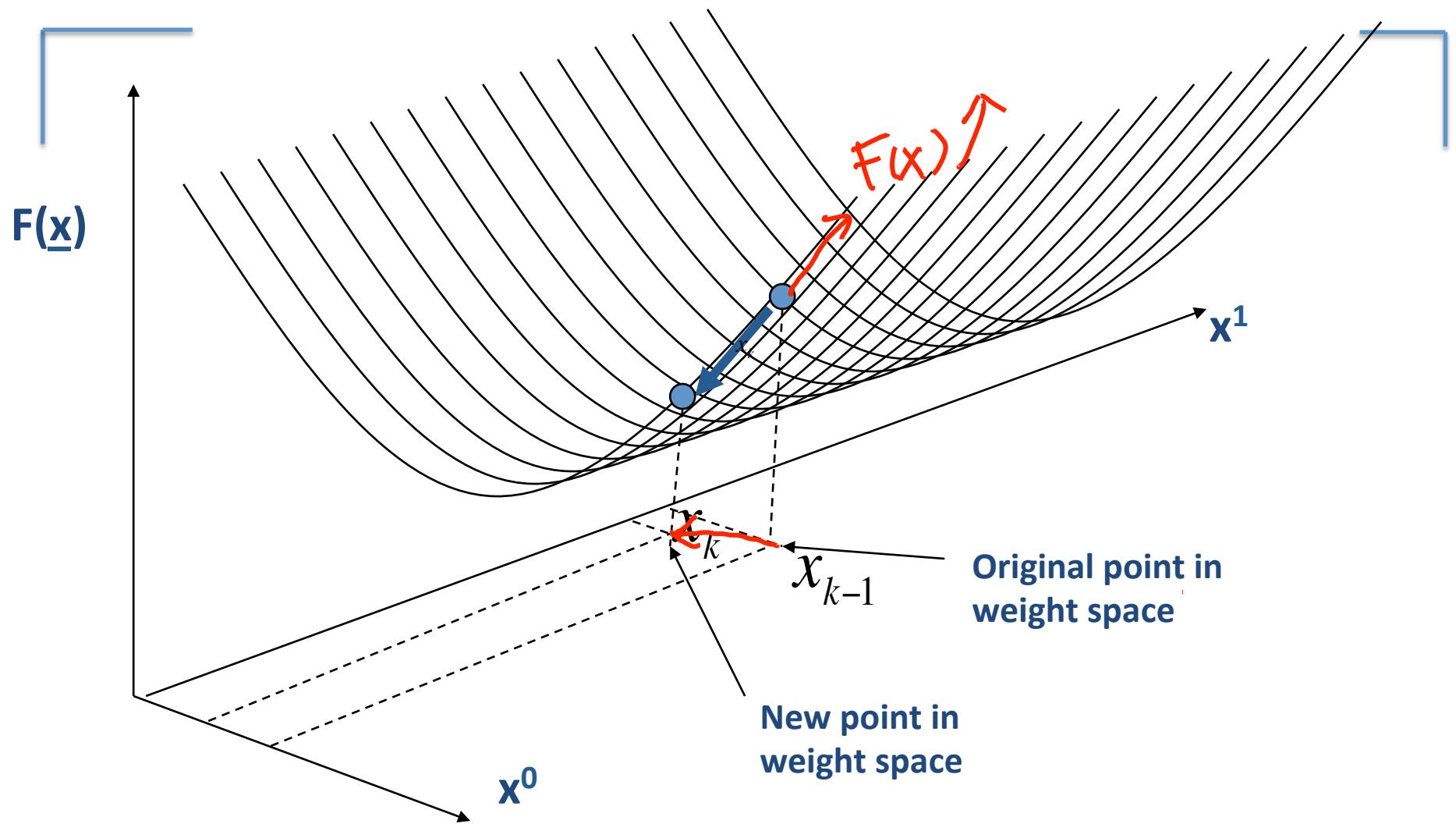
←

$$y'' = 2$$



This convex function is minimized @ the unique point whose derivative (slope) is zero.
→ If finding zeros of the derivative of this function, we can also find minima (or maxima) of that function.

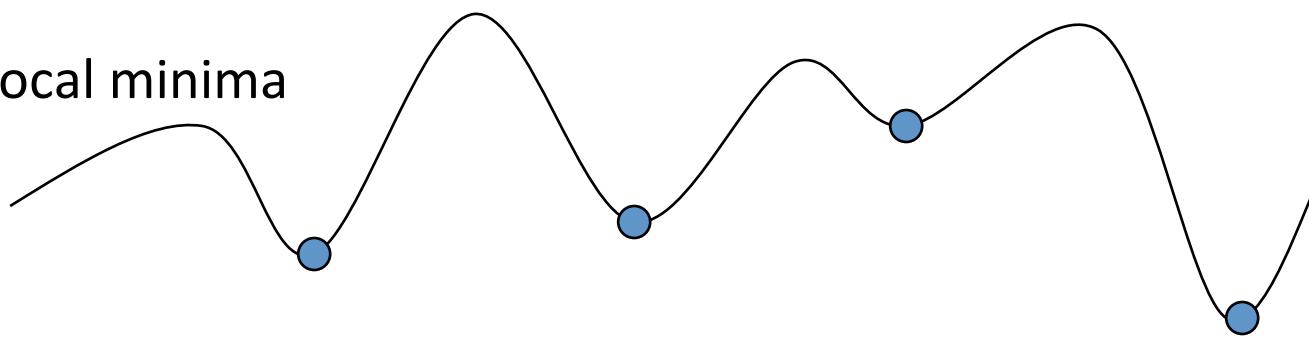
Illustration of Gradient Descent (2D case)



Comments on Gradient Descent Algorithm

- Works on any objective function $F(x)$
 - as long as we can evaluate the gradient
 - this can be very useful for minimizing complex functions

- Local minima



- Can have multiple local minima
- (note: for LR, its cost function only has a single global minimum, so this is not a problem)
- If gradient descent goes to the closest local minimum:
 - solution: random restarts from multiple places in weight space

Today

- ❑ A Practical Application of Regression Model
- ❑ More ways to train / perform optimization for linear regression models
 - ❑ Gradient Descent
 - ❑ Gradient Descent (GD) for LR
 - ❑ Stochastic GD (SGD)
 - ❑ Newton's method

Review: Normal Equation based on Convex loss function

- Intuitively, a convex function has a **single point at which the derivative goes to zero**, and this point is a minimum.

$$J(\theta) = \frac{1}{2} \sum_{i=1}^n (f(\mathbf{x}_i) - y_i)^2$$

- To minimize $J(\theta)$, take derivative and set to zero:

$$\Rightarrow X^T X \theta = X^T \bar{y}$$

The normal equations

$$\theta^* = (X^T X)^{-1} X^T \bar{y}$$

LR with batch GD

- The Cost Function:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i^T \theta - y_i)^2$$

$$\theta_{k+1} = \theta_k - \alpha \nabla_{\theta} J(\theta_k)$$

- Consider a **gradient descent** algorithm:

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_{p-1} \end{bmatrix}$$

$$\theta^{t+1} = \theta^t + \alpha \sum_{i=1}^n (y_i - \mathbf{x}_i^T \theta^t) \mathbf{x}_i$$

$$\theta_j^{t+1} = \theta_j^t - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \Big|_t$$

For the (t+1)-th epoch

$$= \theta_j^t + \alpha \sum_{i=1}^n (y_i - \bar{\mathbf{x}}_i^T \theta^t) x_i^j$$

$J(\theta) = (\mathbf{x}\theta - \mathbf{y})^T (\mathbf{x}\theta - \mathbf{y}) \frac{1}{2}$

$$= ((\mathbf{x}\theta)^T - \mathbf{y}^T)(\mathbf{x}\theta - \mathbf{y}) \frac{1}{2}$$

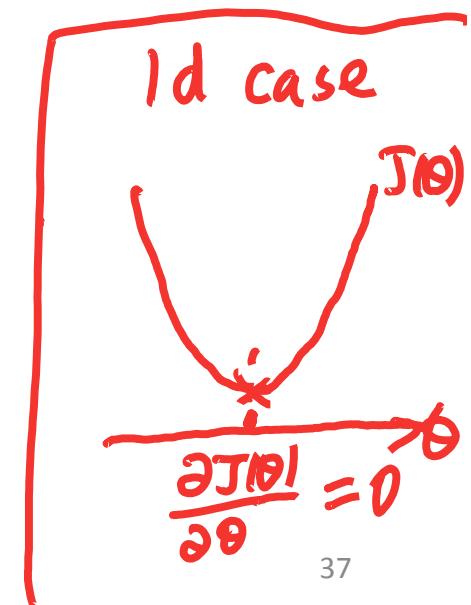
$$= (\theta^T \mathbf{x}^T - \mathbf{y}^T)(\mathbf{x}\theta - \mathbf{y}) \frac{1}{2}$$

$$= (\underbrace{\theta^T \mathbf{x}^T \mathbf{x}\theta - \theta^T \mathbf{x}^T \mathbf{y} - \mathbf{y}^T \mathbf{x}\theta + \mathbf{y}^T \mathbf{y}}_{\text{since } \theta^T \mathbf{x}^T \mathbf{y} = \mathbf{y}^T \mathbf{x}\theta}) \frac{1}{2}$$

$$\langle \mathbf{x}\theta, \mathbf{y} \rangle \quad \langle \mathbf{y}, \mathbf{x}\theta \rangle$$

$$= (\underbrace{\theta^T \mathbf{x}^T \mathbf{x}\theta}_{\text{1d case}} - \underbrace{2\theta^T \mathbf{x}^T \mathbf{y}} + \mathbf{y}^T \mathbf{y}) \frac{1}{2}$$

$\Rightarrow J(\theta)$ quadratic func of θ ;



See handout 4.1 + 4.3 \Rightarrow matrix calculus, partial dari \Rightarrow Gradient

$$\nabla_{\theta} (\theta^T \mathbf{X}^T \mathbf{X} \theta) = 2 \mathbf{X}^T \mathbf{X} \theta \quad (\text{P24})$$

$$\nabla_{\theta} (-2 \theta^T \mathbf{X}^T \mathbf{y}) = -2 \mathbf{X}^T \mathbf{y} \quad (\text{P24})$$

$$\nabla_{\theta} (\mathbf{y}^T \mathbf{y}) = 0$$

$$\Rightarrow \nabla_{\theta} J(\theta) = \boxed{\mathbf{X}^T \mathbf{X} \theta - \mathbf{X}^T \mathbf{y}}$$

$$\nabla_{\theta} J(\theta) = \mathbf{X}^T \mathbf{X} \theta - \mathbf{X}^T \mathbf{Y}$$

$$= \mathbf{X}^T (\underline{\mathbf{X}\theta - \mathbf{Y}})$$

$$= \sum \left(\begin{bmatrix} -x_1^T - \\ -x_2^T - \\ \vdots \\ -x_n^T - \end{bmatrix}_{n \times p} \theta - \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \right)_{p \times 1}$$

$$= \sum_{p \geq 1} \begin{bmatrix} x_1^T \theta - y_1 \\ x_2^T \theta - y_2 \\ \dots \\ x_n^T \theta - y_n \end{bmatrix}_{n \times 1} = \boxed{\begin{bmatrix} 1 & 1 & 1 & \dots & x_1^T \theta - y_1 \\ x_1 & x_2 & \dots & x_n & : \\ 1 & 1 & 1 & \dots & x_n^T \theta - y_n \end{bmatrix}} \quad \boxed{(x_i)}$$

$$= \sum_{i=1}^n x_i \underbrace{(x_i^T \theta - y_i)}_{(x_i)}$$

$$\nabla_{\theta} J(\theta) = \mathbf{X}^T \mathbf{X} \theta - \mathbf{X}^T \mathbf{Y}$$

$$= \mathbf{X}^T (\mathbf{X}\theta - \mathbf{Y})$$

$$= \sum \left(\begin{bmatrix} -x_1^T - \\ -x_2^T - \\ \vdots \\ -x_n^T - \end{bmatrix} \theta - \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \right)$$

$n \times p$ $p \times 1$

$$\mathbf{X} = \begin{bmatrix} \cdots & \mathbf{x}_1^T & \cdots \\ \cdots & \mathbf{x}_2^T & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & \mathbf{x}_n^T & \cdots \end{bmatrix}$$

$$= \sum_{p \geq 1} \begin{bmatrix} x_1^T \theta - y_1 \\ x_2^T \theta - y_2 \\ \vdots \\ x_n^T \theta - y_n \end{bmatrix}_{n \times 1} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n & \end{bmatrix} \begin{bmatrix} x_1^T \theta - y_1 \\ x_2^T \theta - y_2 \\ \vdots \\ x_n^T \theta - y_n \end{bmatrix}$$

$$= \sum_{i=1}^n x_i \cdot \boxed{(x_i^T \theta - y_i)}$$

1 * 1



LR with batch GD

- Steepest descent / GD
 - Note that:

$$\nabla_{\theta} J = \left[\frac{\partial}{\partial \theta_1} J, \dots, \frac{\partial}{\partial \theta_k} J \right]^T = - \sum_{i=1}^n (y_i - \mathbf{x}_i^T \theta) \mathbf{x}_i$$

Based on Handout's
Definition of
Gradient
(Denominator)

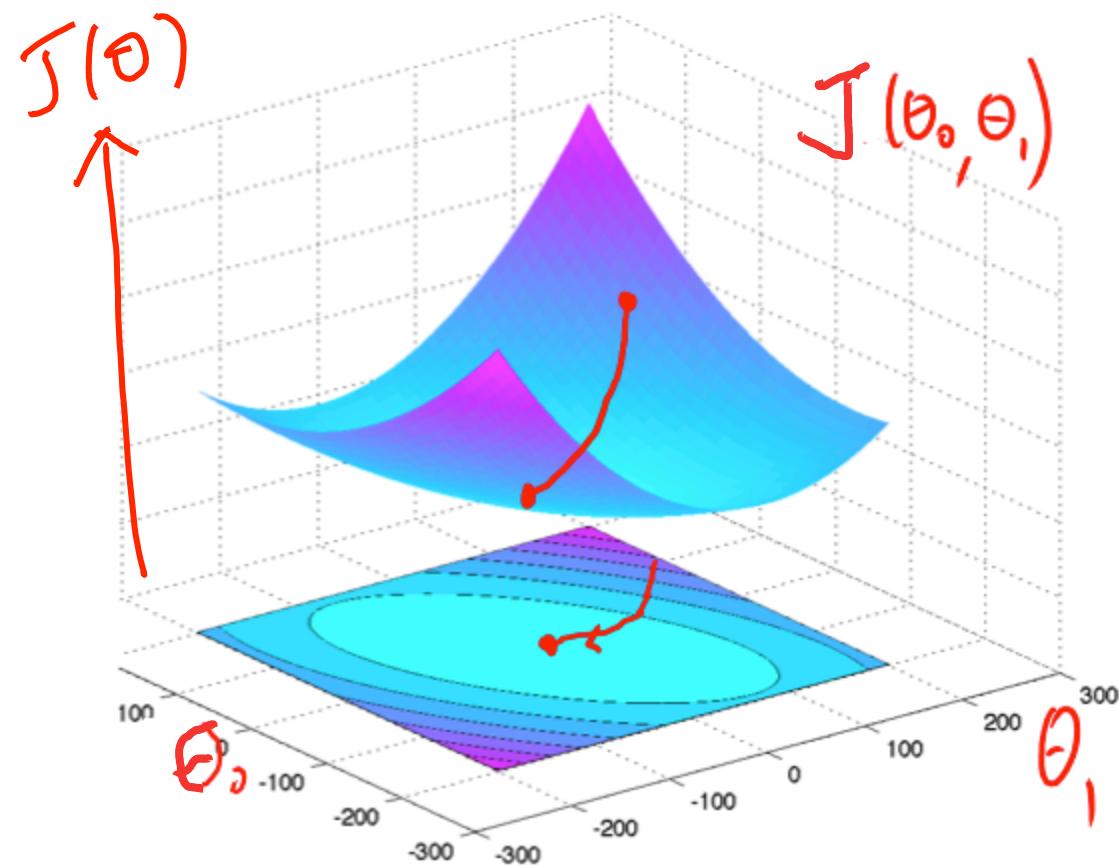
$$\theta^{t+1} = \theta^t + \alpha \sum_{i=1}^n (y_i - \mathbf{x}_i^T \theta^t) \mathbf{x}_i$$

– This is as a **batch** gradient descent algorithm

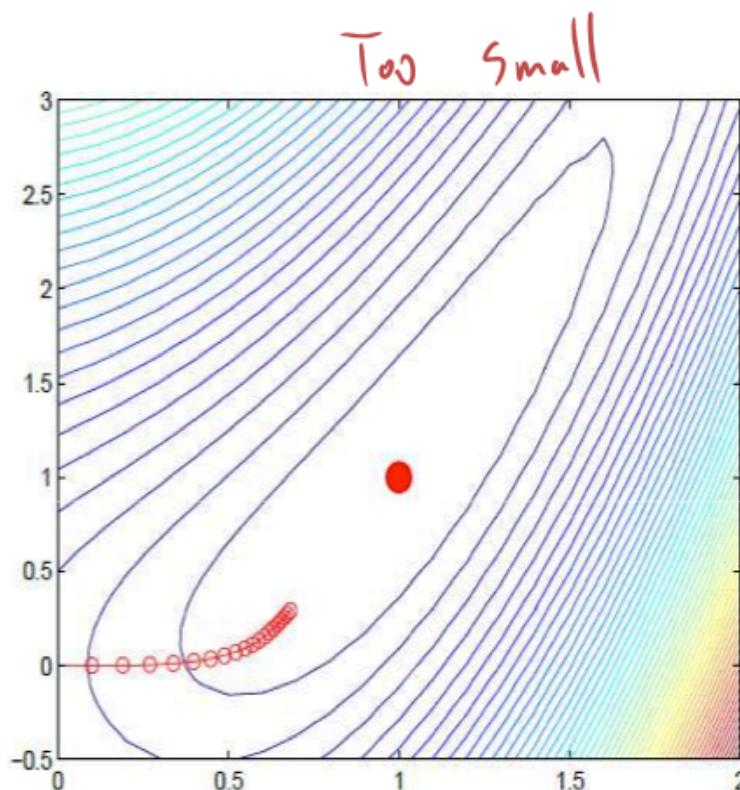
$$\theta_j^{t+1} = \theta_j^t + \alpha \sum_{i=1}^n (y_i - \bar{\mathbf{x}}_i^T \theta^t) x_i^j$$

Update Rule Per
Feature
(Variable-Wise)

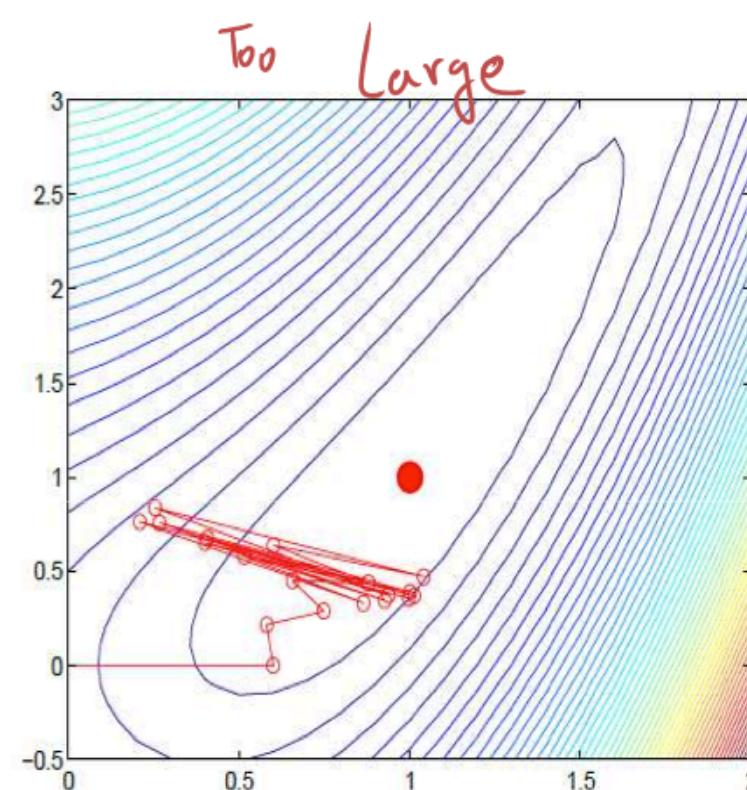
Illustration of Gradient Descent (2D case)



Choosing the Right Step-Size / Learning-Rate is critical



$$\alpha = 0.1.$$



$$\alpha = 0.6.$$

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 - ❑ Newton's method

LR with Stochastic GD →

- Batch GD rule:

$$\theta^{t+1} = \theta^t + \alpha \sum_{i=1}^n (y_i - \bar{\mathbf{x}}_i^T \theta^t) \bar{\mathbf{x}}_i$$

- Therefore, for a single training point (i-th), we have:

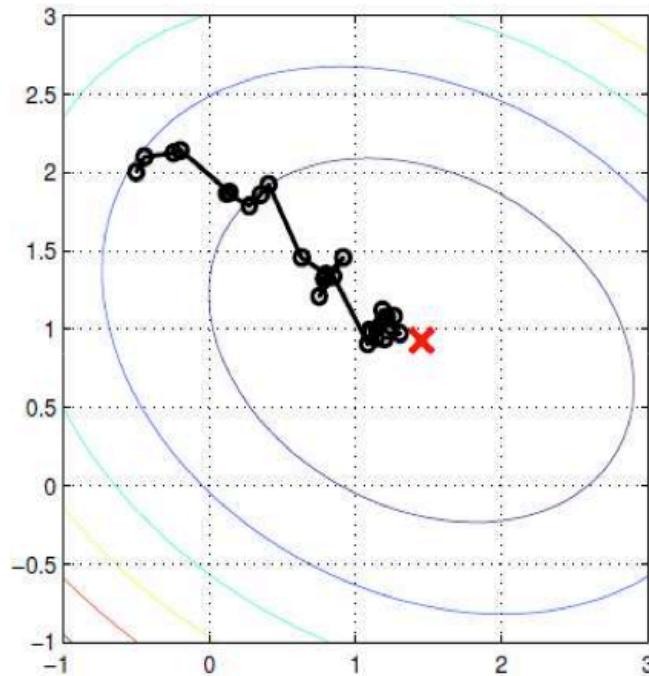
$$\theta^{t+1} = \theta^t + \alpha (y_i - \bar{\mathbf{x}}_i^T \theta^t) \bar{\mathbf{x}}_i$$

$$\theta_j^{t+1} = \theta_j^t + \alpha (y_i - \bar{\mathbf{x}}_i^T \theta^t) x_{i,j}$$

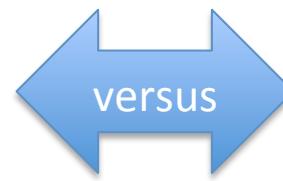
- This is actually a "**stochastic**", "**coordinate**" descent algorithm
- This can be used as an **on-line** algorithm

Stochastic gradient descent / Online Learning Algorithm

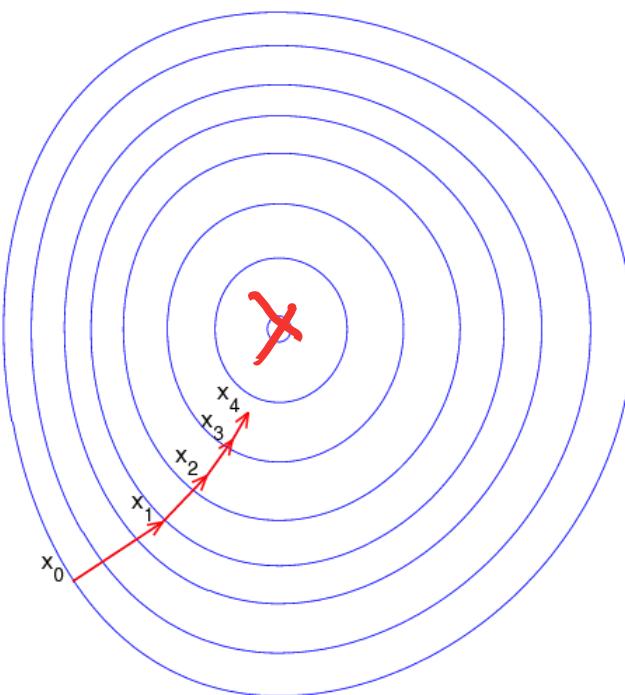
SGD



GD



versus



Stochastic gradient descent : More variations

- Single-sample:

$$\theta^{t+1} = \theta^t + \alpha (y_i - \vec{X}_i^T \theta^t) \vec{X}_i$$

- Mini-batch:

$$\theta^{t+1} = \theta^t + \alpha \sum_{j=1}^B (y_j - \vec{X}_j^T \theta^t) \vec{X}_j$$

e.g. $B=15$

Stochastic gradient descent (1)

- Very useful when training with massive datasets , e.g. not fit in main memory
- SGD can be used for offline training, by repeated cycling through the data
 - Each such pass over the whole data → an epoch !
- In offline case, often better to use mini-batch SGD
 - $B=1$ standard SGD
 - $B=N$ standard batch GD
 - E.g. $B=100$

① Massive Data

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Stochastic gradient descent (2)

②

Intuitively, one can get a fairly good estimate of the gradient by looking at just a few examples. Carefully evaluating precise gradients using large datasets is often a waste of time, since the algorithm will have to recompute the gradient again anyway at the next step. It is often a better use of computer time to have a noisy estimate and to move rapidly through parameter space.

③

SGD is often less prone to getting stuck in shallow local minima, because it adds a certain amount of "noise". Consequently it is quite popular in the machine learning community for fitting models such as neural networks and deep belief networks with non-convex objectives.

When to stop (S)GD ?

- Lots of stopping rules in the literature,
- There are advantages and disadvantages to each, depending on context
- E.g., a predetermined maximum number of iterations
- E.g., stop when the improvement drops below a threshold
-

Summary so far: three ways to learn LR

- Normal equations

$$\theta^* = (X^T X)^{-1} X^T \bar{y}$$

$\mathcal{O}(n p^2) + \mathcal{O}(p^3)$

- Pros: a single-shot algorithm! Easiest to implement.
- Cons: need to compute pseudo-inverse $(X^T X)^{-1}$, expensive numerical issues (e.g., matrix is singular ..), although there are ways to get around this
...

- GD or Steepest descent

$$\theta^{t+1} = \theta^t + \alpha \sum_{i=1}^n (y_i - \mathbf{x}_i^T \theta^t) \mathbf{x}_i$$

- Pros: easy to implement, conceptually clean, guaranteed convergence
- Cons: batch, often slow converging

- Stochastic GD

$$\theta^{t+1} = \theta^t + \alpha (y_i - \bar{\mathbf{x}}_i^T \theta^t) \bar{\mathbf{x}}_i$$

- Pros: on-line, low per-step cost, fast convergence and perhaps less prone to local optimum
- Cons: convergence to optimum not always guaranteed

Direct (normal equation) vs. Iterative (GD) methods

- **Direct methods:** we can achieve the solution in a single step by solving the normal equation
 - Using Gaussian elimination or QR decomposition, we converge in a finite number of steps
 - It can be infeasible when data are streaming in real time, or of very large amount
- **Iterative methods:** stochastic or steepest gradient
 - Converging in a limiting sense
 - But more attractive in large practical problems
 - Caution is needed for deciding the learning rate

Scale up to big n or big p ?

Given: A labeled training set, $\{x_i, y_i\}_{i=1\dots n}$ $x_i \in \mathbb{R}^d, y_i \in \mathbb{R}$
 $n \sim O(100M), d \sim O(100K)$

Goal: Learn a predictive function $f(x; w) = w^T x + w_0$

$$\hat{w} = \underbrace{(XX^T + \lambda I)^{-1}}_{O(nd^2)} Xy \underbrace{\quad}_{O(d^3)}$$

$n \sim O(100M), d \sim O(100K)$

Matrix multiplication is slower than inversion!
 Matrix inversion is intractable!
 First-order linear solvers $Aw = b$?

But this is just linear !

Dr. Sanjay Kumar slide

Convergence rate

- **Theorem:** the steepest descent equation algorithm converge to the minimum of the cost characterized by normal equation:

$$\theta^{(\infty)} = (X^T X)^{-1} X^T y$$

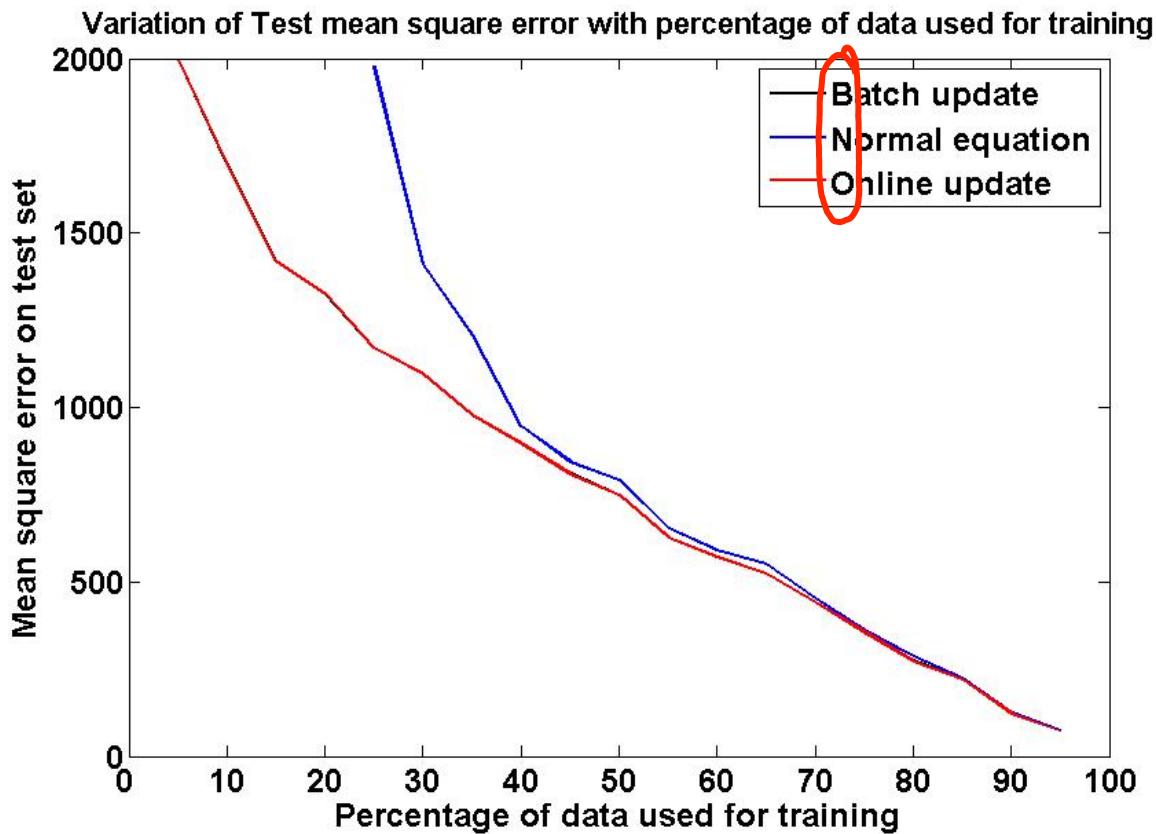
If the learning rate parameter satisfy →

$$0 < \alpha < 2/\lambda_{\max}[X^T X]$$

- A formal analysis of GD-LR need more math; in practice, one can use a small α , or gradually decrease α .

$$\alpha_0 = 0.05$$

Performance vs. Training Size for an example



- The results from B and O update are almost identical. So the plots coincide.
- The test MSE from the normal equation is more than that of B and O during small training. This is probably due to overfitting.
- In B and O, since only 2000 (for example) iterations are allowed at most. This roughly acts as a mechanism that avoids overfitting.

Today

- ❑ A Practical Application of Regression Model
- ❑ More ways to train / perform optimization for linear regression models
 - ❑ Gradient Descent
 - ❑ Gradient Descent (GD) for LR
 - ❑ Stochastic GD (SGD)
 - ❑ Newton's method

Review: Convex function

- Intuitively, a convex function (1D case) has a single point at which the derivative goes to zero, and this point is a minimum.
- Intuitively, a function f (1D case) is convex on the range $[a,b]$ if a function's second derivative is positive every-where in that range.
- Intuitively, if a function's Hessians is psd (positive semi-definite!), this (multivariate) function is Convex
 - Intuitively, we can think “Positive definite” matrices as analogy to positive numbers in matrix case

Newton's method for optimization

- The most basic **second-order** optimization algorithm
- Updating parameter with

$$\text{Newton: } \theta_{k+1} = \theta_k - H_K^{-1} g_k$$

$$\text{GD: } \theta_{k+1} = \theta_k - \alpha g_k$$

$\underbrace{P \times P \quad P \times 1}_{P \times 1}$

Review: Hessian Matrix / n==2 case

Singlevariate \rightarrow multivariate

$$f(x, y)$$

- 1st derivative to gradient,

$$g = \nabla f = \begin{pmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{pmatrix}$$

- 2nd derivative to Hessian

$$H = \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{pmatrix}$$

Review: Hessian Matrix

Suppose that $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is a function that takes a vector in \mathbb{R}^n and returns a real number. Then the **Hessian** matrix with respect to x , written $\nabla_x^2 f(x)$ or simply as H is the $n \times n$ matrix of partial derivatives,

$$\nabla_x^2 f(x) \in \mathbb{R}^{n \times n} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}.$$

Newton's method for optimization

- Making a quadratic/second-order Taylor series approximation

$$\hat{f}_{quad}(\boldsymbol{\theta}) = f(\boldsymbol{\theta}_k) + \mathbf{g}_k^T (\boldsymbol{\theta} - \boldsymbol{\theta}_k) + \frac{1}{2} (\boldsymbol{\theta} - \boldsymbol{\theta}_k)^T \mathbf{H}_k (\boldsymbol{\theta} - \boldsymbol{\theta}_k)$$

Finding the minimum solution of the above right quadratic approximation (quadratic function minimization is easy !)

$$\hat{f}(\theta) = f(\theta_K) + g_K^\top (\theta - \theta_K) + \frac{1}{2} (\theta - \theta_K)^\top H_K (\theta - \theta_K)$$

$\frac{1}{2} (\theta^\top H_K \theta - 2\theta^\top H_K \theta_K + \theta_K^\top H_K \theta_K)$

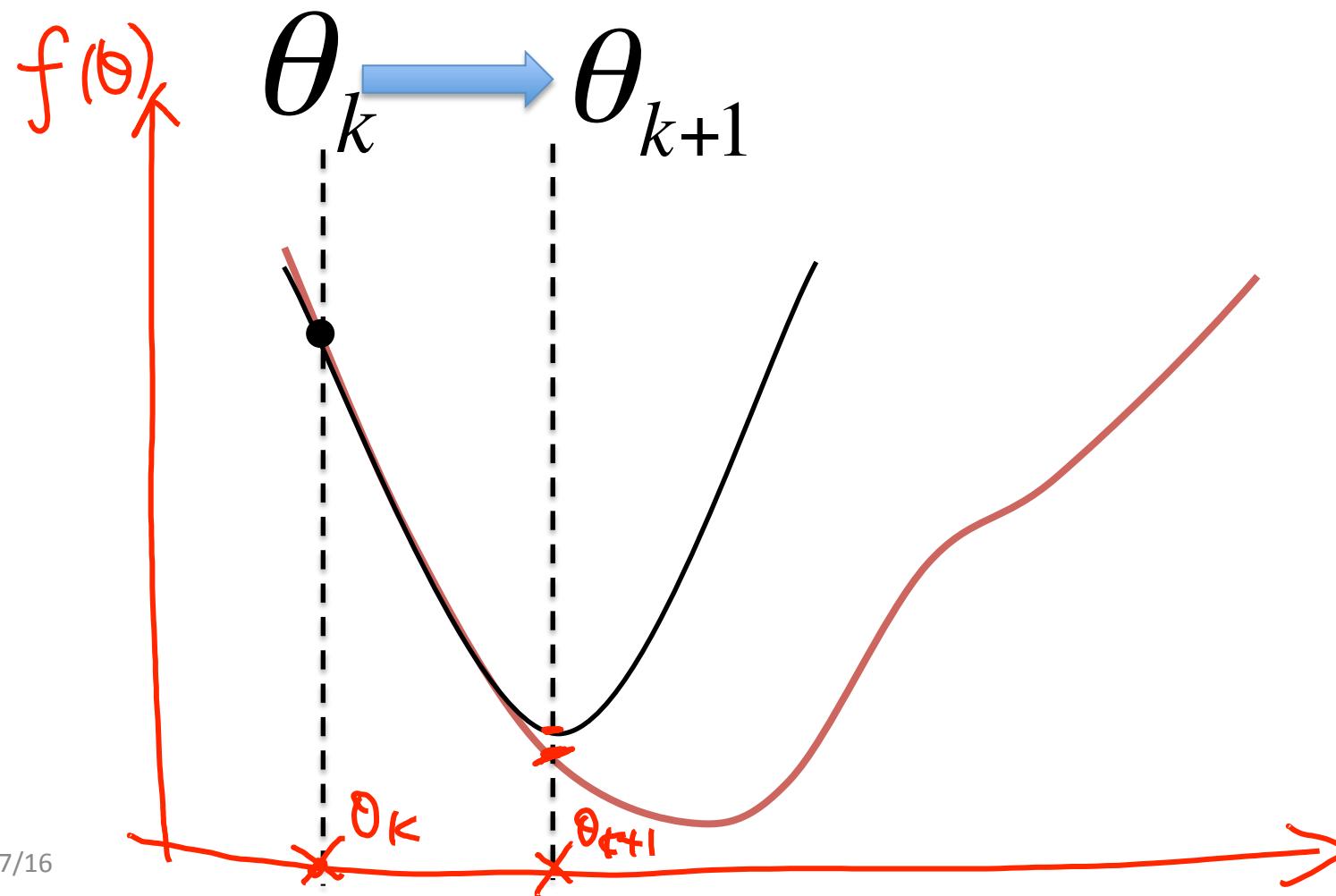
$$\frac{\partial \hat{f}(\theta)}{\partial \theta} = 0 + g_K + \underbrace{\frac{2}{2} H_K \theta - \frac{2}{2} H_K \theta_K}_{\text{see p24 handout}} := 0$$

$$g_K + H_K (\theta - \theta_K) = 0$$

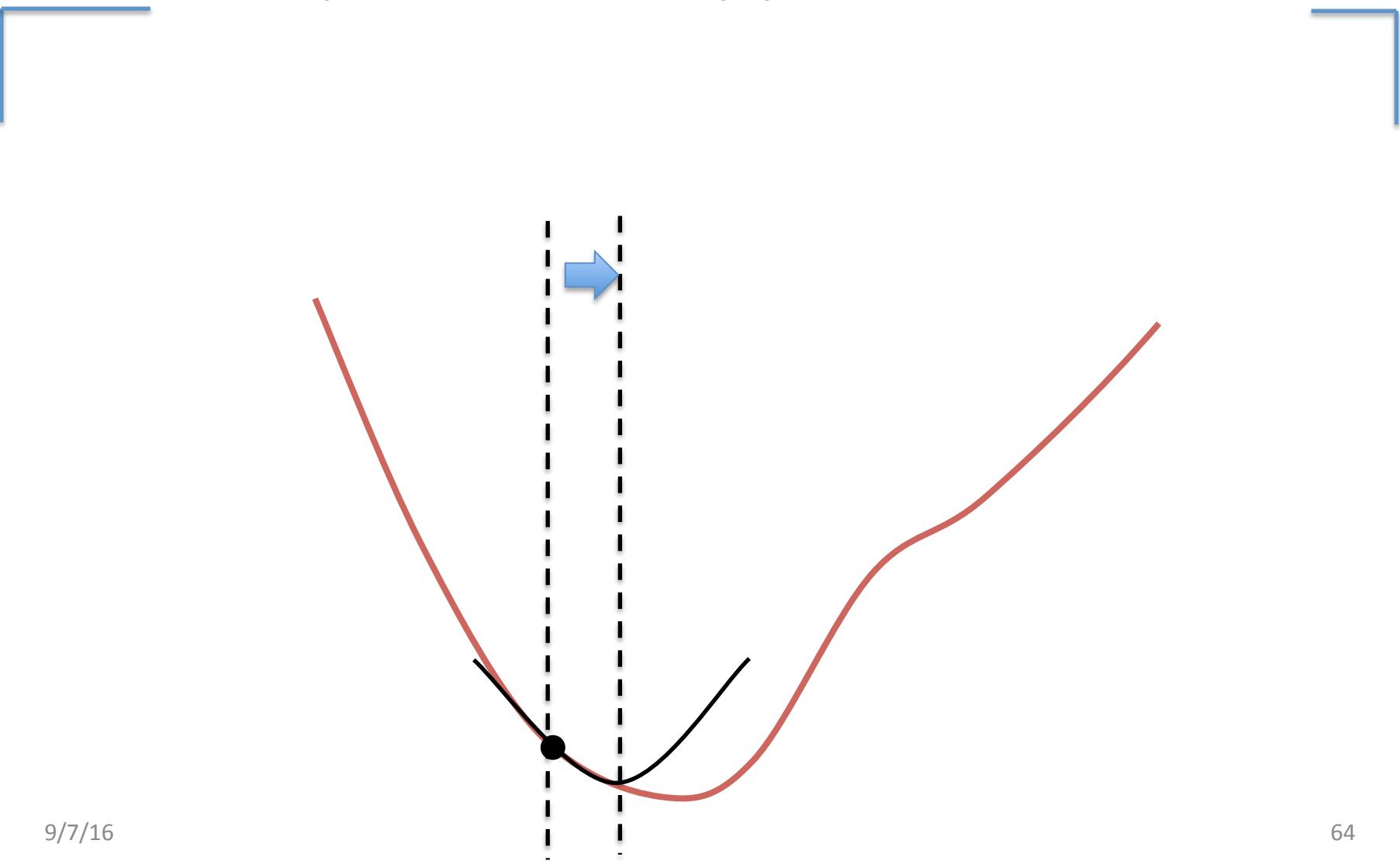
$$\Rightarrow \theta = \theta_K - H_K^{-1} g_K \quad \begin{matrix} \text{where } H_K \in \mathbb{R}^{P \times P} \\ \text{if } g_K \in \mathbb{R}^P \end{matrix}$$

Newton's Method / second-order Taylor series approximation

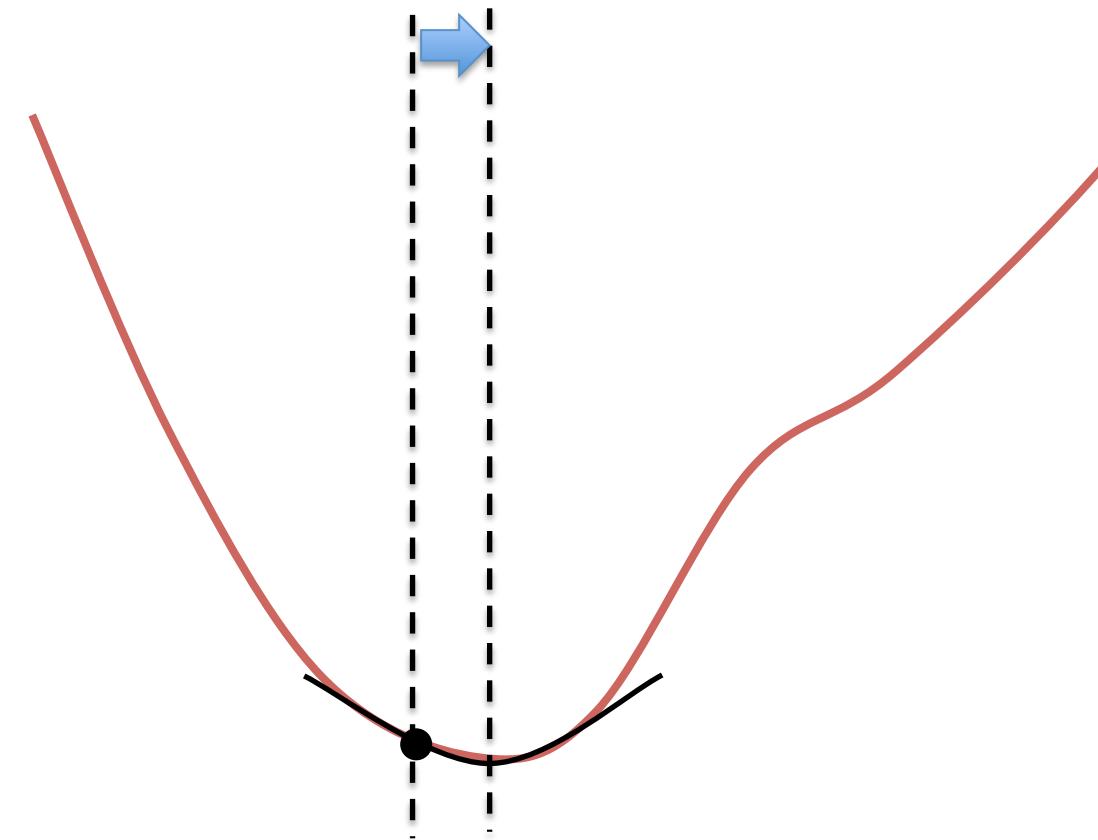
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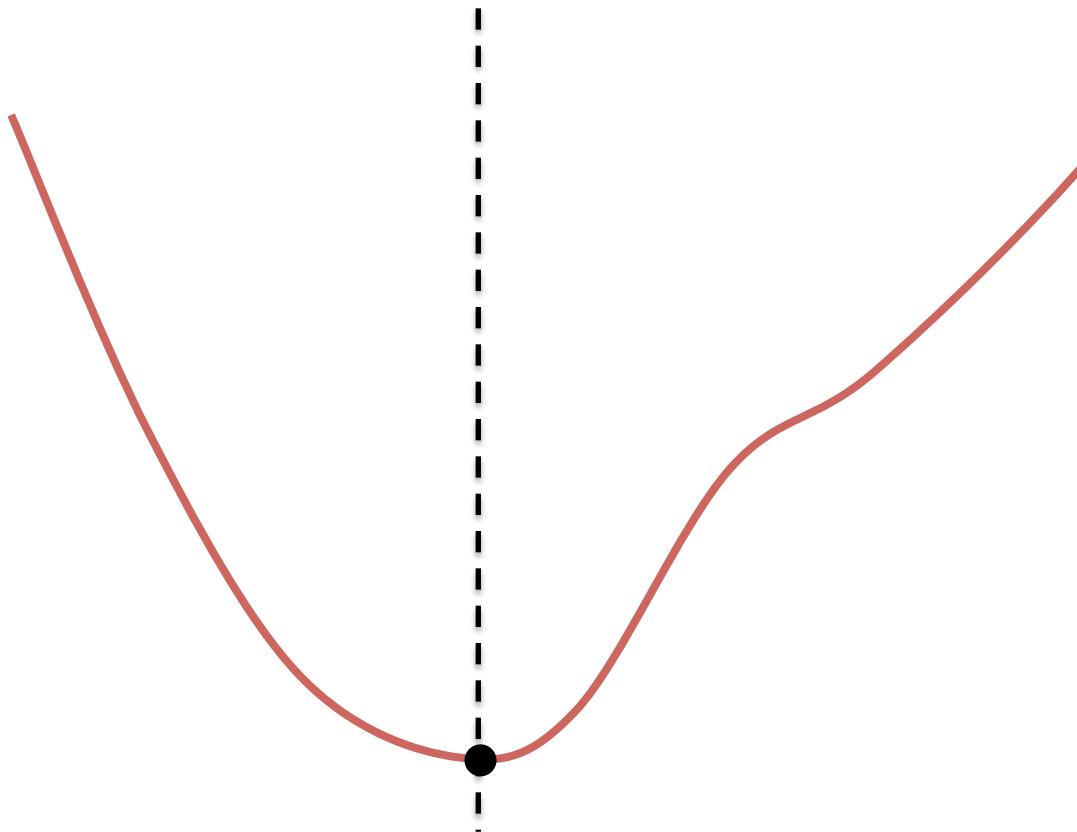
Newton's Method / second-order Taylor series approximation



Newton's Method / second-order Taylor series approximation



Newton's Method / second-order Taylor series approximation



Newton's Method

- At each step:

$$\theta_{k+1} = \theta_k - \frac{f'(\theta_k)}{f''(\theta_k)}$$

$$\theta_{k+1} = \theta_k - H^{-1}(\theta_k) \nabla f(\theta_k)$$

- Requires 1st and 2nd derivatives
- Quadratic convergence
- → However, finding the inverse of the Hessian matrix is often expensive

Newton vs. GD for optimization

- **Newton:** a quadratic/second-order Taylor series approximation

$$\Theta_{k+1} = \Theta_k - \frac{1}{H(\Theta_k)} g(\Theta_k)$$

$$\hat{f}_{quad}(\theta) = f(\theta_k) + \mathbf{g}_k^T (\theta - \theta_k) + \frac{1}{2} (\theta - \theta_k)^T \mathbf{H}_k (\theta - \theta_k)$$

- **GD:** a approximation

Finding the minimum solution of the above right quadratic approximation (quadratic function minimization is easy !)

$$\hat{f}_{quad}(\theta) = f(\theta_k) + \mathbf{g}_k^T (\theta - \theta_k) + \frac{1}{2} (\theta - \theta_k)^T \frac{1}{\alpha} (\theta - \theta_k)$$

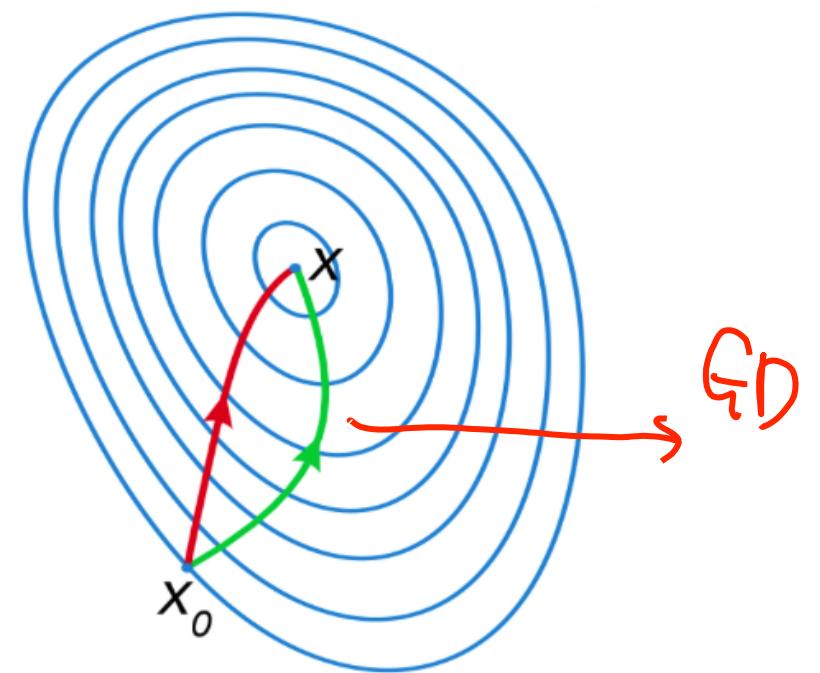
$$\Downarrow \Theta_{k+1} = \Theta_k - \alpha \mathbf{g}(\Theta_k)$$

Comparison

- Newton's method vs. Gradient descent

A comparison of gradient descent (**green**) and Newton's method (**red**) for minimizing a function (with small step sizes).

Newton's method uses curvature information to get a more direct route ...



$$J(\theta) = \frac{1}{2} (\gamma - X\theta)^T (\gamma - X\theta)$$

$$\nabla_{\theta} J(\theta) = X^T X \theta - X^T \gamma$$

$$H = \nabla_{\theta}^2 J(\theta) = X^T X$$

$$\begin{aligned} \Rightarrow \theta^t &= \theta^{t-1} - H^{-1} \nabla J(\theta^{t-1}) \quad \text{Newton} \\ &= \theta^{t-1} - [X^T X]^{-1} [X^T X \theta^{t-1} - X^T \gamma] \\ &= [\theta^{t-1} - \theta^{t-1}] + (X^T X)^{-1} X^T \gamma \\ &= (X^T X)^{-1} X^T \gamma \end{aligned}$$

WHY
???
Normal Eq?

9/7/16

Newton's method
for Linear Regression

Today Recap

- ❑ A Practical Application of Regression Model
- ❑ More ways to train / perform optimization for linear regression models
 - ❑ Gradient Descent
 - ❑ Gradient Descent (GD) for LR
 - ❑ Stochastic GD (SGD)
 - ❑ Newton's method

Evaluation : for Regression Models

$$J(\theta) = \frac{1}{2} \sum_{i=1}^n (\hat{y}_i(\bar{x}_i) - y_i)^2$$

Sum of squared error
(SSE) on training set

- Testing MSE (mean-squared-error) to report:

$$MSE_{test} = \frac{1}{m} \sum_{i=n+1}^{n+m} (\mathbf{x}_i^T \boldsymbol{\theta}^* - y_i)^2$$

- Training MSE to report:

$$MSE_{train} = \frac{1}{n} \sum_{i=1}^n (\mathbf{x}_i^T \boldsymbol{\theta}^* - y_i)^2$$

References

- Big thanks to Prof. Eric Xing @ CMU for allowing me to reuse some of his slides
 - **Notes about Gradient Descent from Toussaint:** <http://ipvs.informatik.uni-stuttgart.de/mlr/marc/notes/gradientDescent.pdf>
 - http://en.wikipedia.org/wiki/Matrix_calculus
 - Prof. Nando de Freitas's tutorial slide