Least Squares Optimization and Gradient Descent Algorithm

Example

- Single Variable Linear Regression

estimate $\hat{y}_i = \theta_0 + \theta_1 x_i$

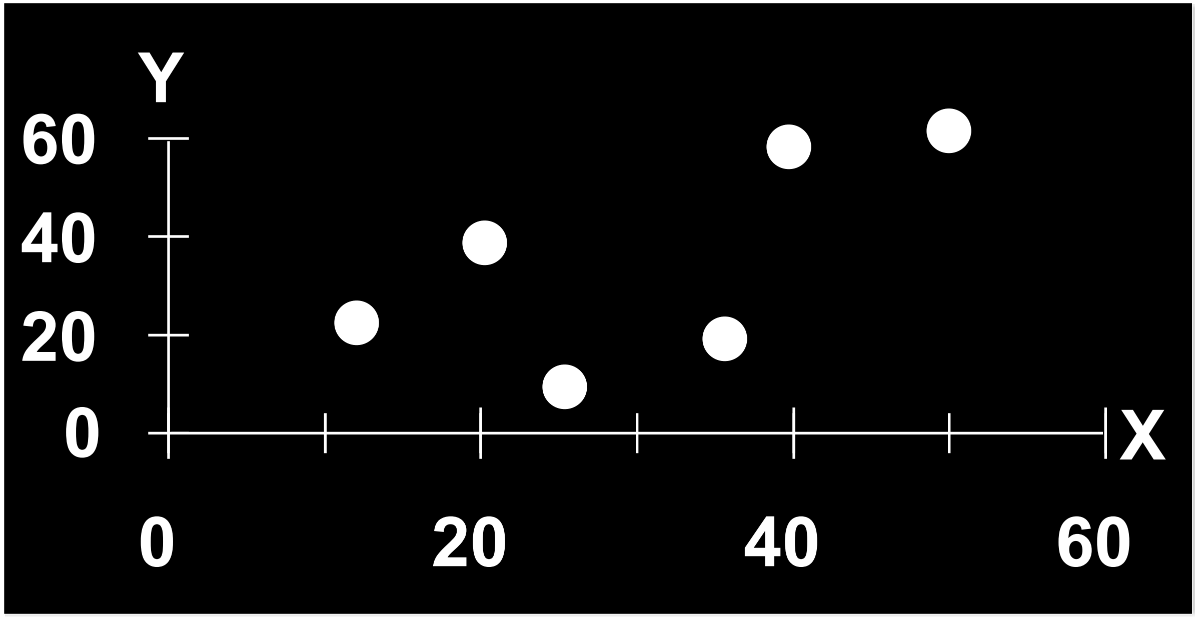
x	y
12	20
20	40
25	10
35	20
40	60
50	65

?

ESTIMATING PARAMETERS: LEAST SQUARES METHOD

SCATTER PLOT

Plot all (X_i, Y_i) pairs, and plot your learned model



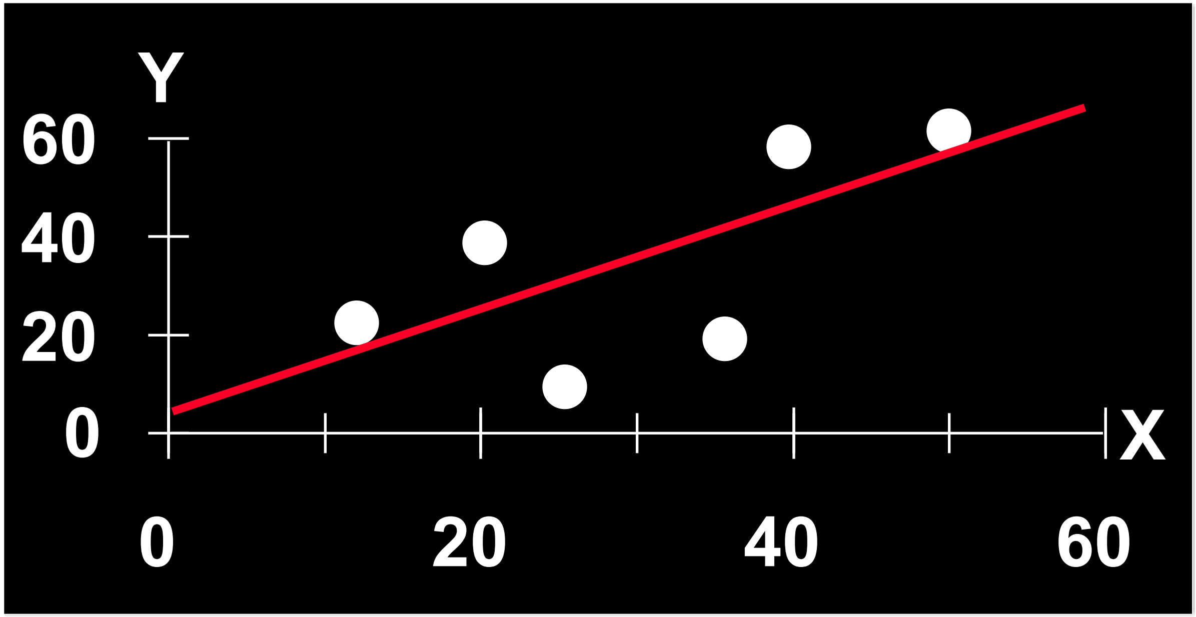
[WF]

QUESTION

How would you draw a line through the points?

How do you determine which line “fits the best” …?

??????????



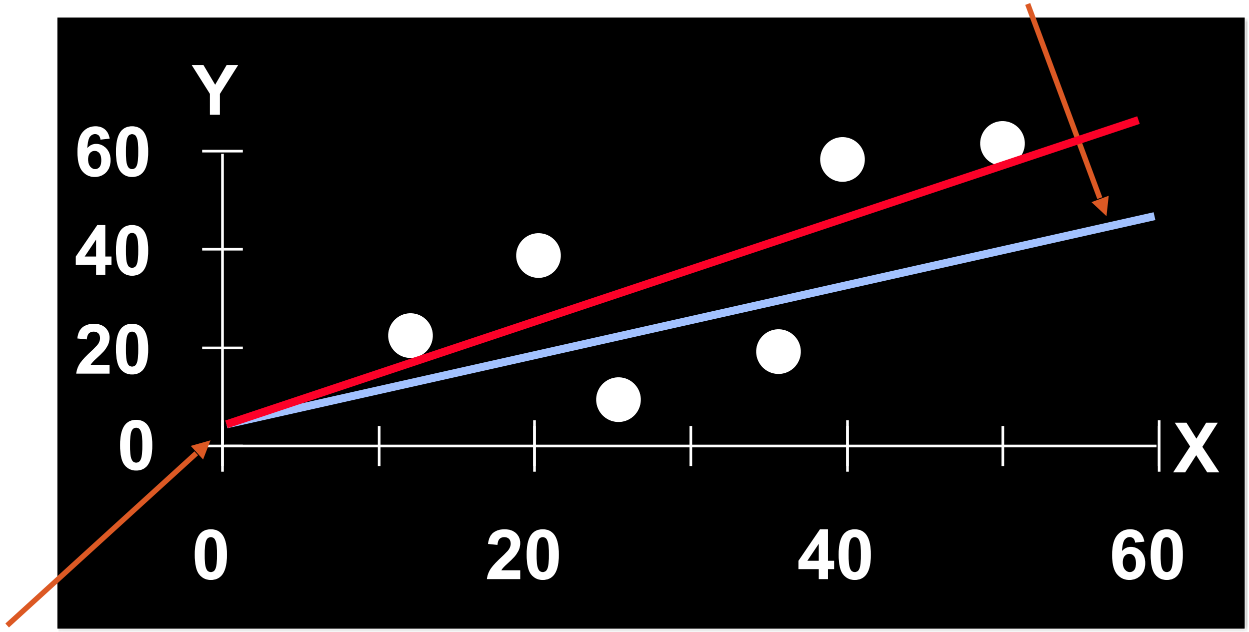
[WF]

QUESTION

How would you draw a line through the points?

How do you determine which line “fits the best” ?????????

Slope changed



Intercept unchanged

[WF]

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How would you draw a line through the points?

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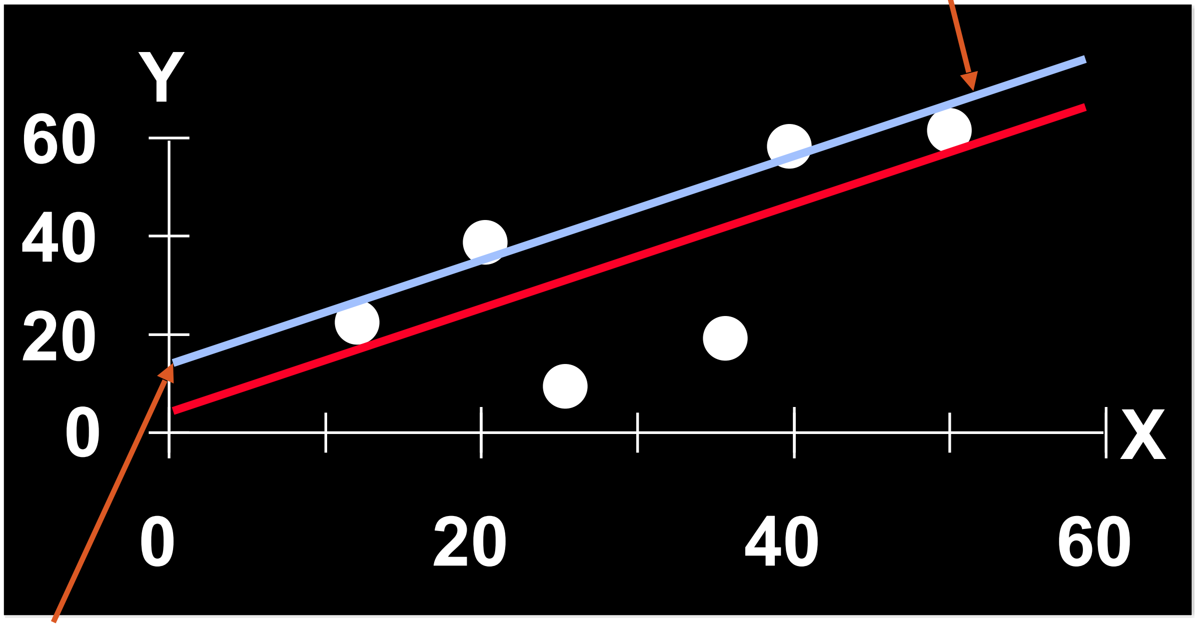
Slope unchanged



Intercept changed

[WF]

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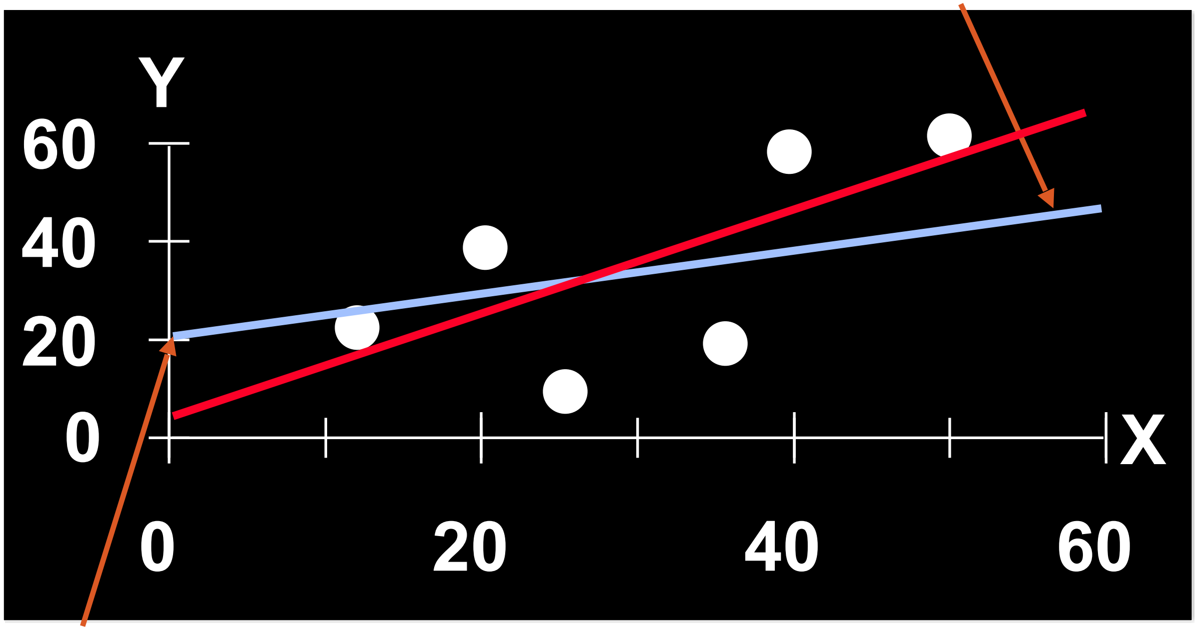


Intercept changed

LEAST SQUARES

Best fit: difference between the true (observed) Y-values and the estimated Y-values is minimized:

- Positive errors offset negative errors …
- … square the error!

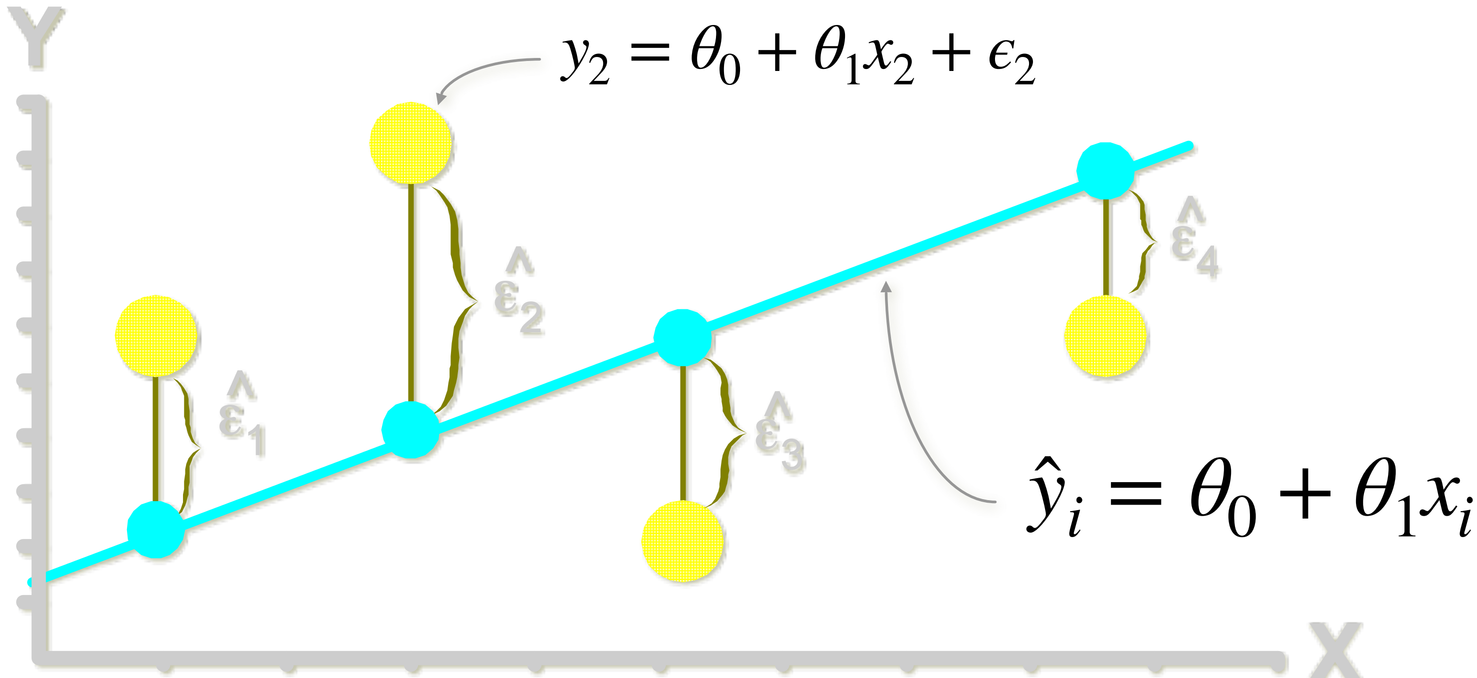
$$\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \epsilon_i^2$$

Least squares minimizes the sum of the squared errors

[WF]

LEAST SQUARES, GRAPHICALLY

LS Minimizes $\sum_{i=1}^{n} \epsilon_i^2 = \epsilon_1^2 + \epsilon_2^2 + \ldots + \epsilon_n^2$



[WF]

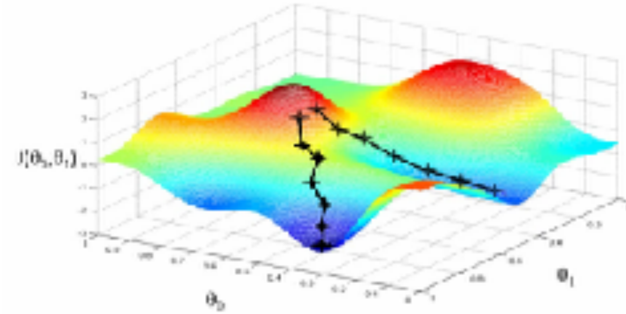
Example

- Single Variable Linear Regression

estimate $\hat{y}_i = \theta_0 + \theta_1 x_i$

x Area(sq. ft.)	y Price (in 1000$)
1600	220
1400	180
2100	350
…	…
….	….
2400	500

Multivariate Regression

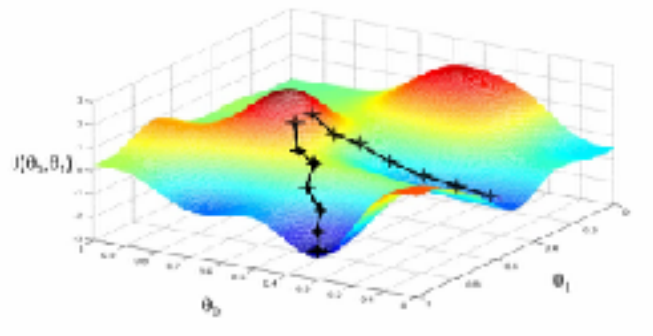


- Multi Linear Regression

$$\hat{y}_i = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2} + \ldots + \theta_m x_{im}$$

y Price (in 1000$)	x_1 Area(sq. ft.)	x_2 # Bathrooms	x_3 # Bedrooms
220	1600	2.5	3
180	1400	1.5	3
350	2100	3.5	4
…	…	…	…
….	….	…	…
500	2400	4	5

Multivariate Regression



- Multi Linear Regression

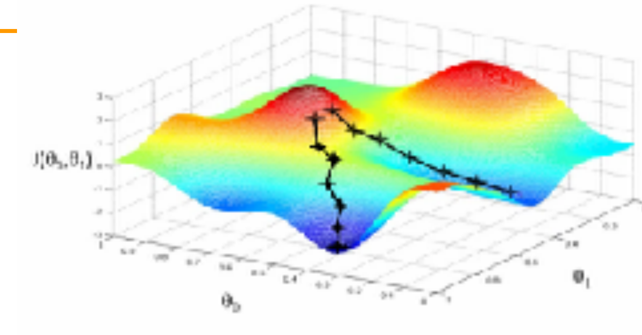
$$\hat{y}_i = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2} + \ldots + \theta_m x_{im}$$

	Price (in 1000$)	Area(sq. ft.)	# Bathrooms	# Bedrooms
	220	1600	2.5	3
yi	180	1400	1.5	3
	350	2100	3.5	4
	…	…	…	…
	….	….	…	…
	500	2400	4	5

x_i

1400	x_{i1}
1.5	x_{i2}
3	x_{i3}

Multivariate Regression



- Multi Linear Regression

$$y_i = \theta_0 x_{i0} + \theta_1 x_{i1} + \theta_2 x_{i2} + \ldots + \theta_m x_{im}$$

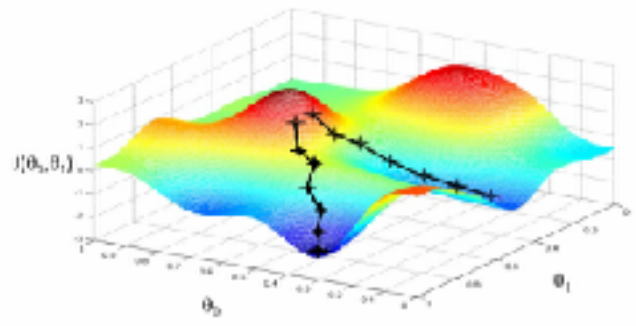
	y	x_0	x_1	x_2	x_3
	Price (in 1000$)		Area(sq. ft.)	# Bathrooms	# Bedrooms
	220	1	1600	2.5	3
y_i	180	1	1400	1.5	3
	350	1	2100	3.5	4
	…	…	…	…	…
	….	….	….	…	…
	500	1	2400	4	5

x_i

1	x_{i0}
1400	x_{i1}
1.5	x_{i2}
3	x_{i3}

Multivariate Regression Model

- Model:



$$\hat{y}_i = \theta_0 x_{i0} + \theta_1 x_{i1} + \theta_2 x_{i2} + \ldots + \theta_m x_{im}$$

$$\hat{y}_i = \sum_{j=0}^{m} \theta_{ij} x_{ij}$$

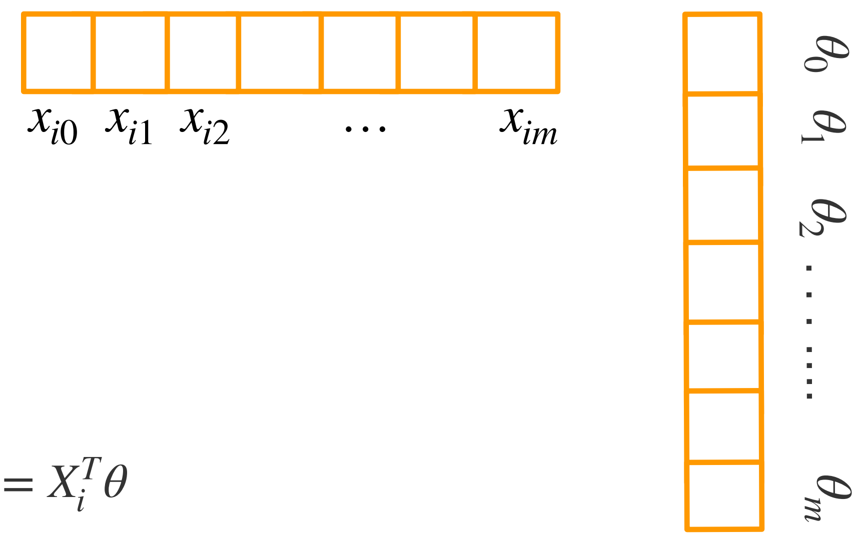
feature 1 = x_0 …. (constant, 1)
feature 2 = x_1 …. (area, sq. ft.)
feature 3 = x_2 …. (# of bedrooms)
feature 4 = x_3 …. (# of bathrooms)
….
….
feature m = x_m

One Observation Model

- Matrix Notation
  For observation i

$$\hat{y}_i = \sum_{j=0}^{m} \theta_{ij} x_{ij}$$

$y_i =$



$$y_i = X_i^T \theta$$

All Observation Model

- Matrix Notation
  For all observations

$$
\begin{bmatrix}
x_{10} & x_{11} & x_{12} & .. & .. & x_{im} \\
x_{20} & x_{21} & x_{22} & .. & .. & x_{2m} \\
x_{30} & x_{31} & x_{32} & .. & .. & x_{3m} \\
. & . & . & . & . & . \\
. & . & . & . & . & . \\
. & . & . & . & . & . \\
x_{n0} & x_{n1} & x_{n2} & .. & .. & x_{nm}
\end{bmatrix}
\begin{bmatrix}
\theta_0 \\ \theta_1 \\ \theta_2 \\ . \\ \theta_m
\end{bmatrix}
=
\begin{bmatrix}
y_0 \\ y_1 \\ y_2 \\ . \\ . \\ . \\ y_n
\end{bmatrix}
$$

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

LEAST SQUARES OPTIMIZATION

Rewrite inputs:

Each row is a feature vector paired with a label for a single input

n labeled inputs

$$X = \begin{bmatrix} (x^{(1)})^T \\ (x^{(2)})^T \\ \cdots \\ (x^{(n)})^T \end{bmatrix} \in \mathbb{R}^{n \times m}, \quad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \cdots \\ y^{(n)} \end{bmatrix} \in \mathbb{R}^n$$

m features

Rewrite optimization problem:

$$\text{minimize}_\theta \ \frac{1}{2} \|X\theta - y\|_2^2$$

*Recall $||z||_2^2 = z^T z = \sum z_i^2$

LEAST SQUARES OPTIMIZATION

Rewrite inputs:

Each row is a feature vector paired with a label for a single input

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$$X = \begin{bmatrix} (x^{(1)})^T \\ (x^{(2)})^T \\ \cdots \\ (x^{(n)})^T \end{bmatrix} \in \mathbb{R}^{n \times m}, y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \cdots \\ y^{(n)} \end{bmatrix} \in \mathbb{R}^n$$

m features

Rewrite optimization problem:

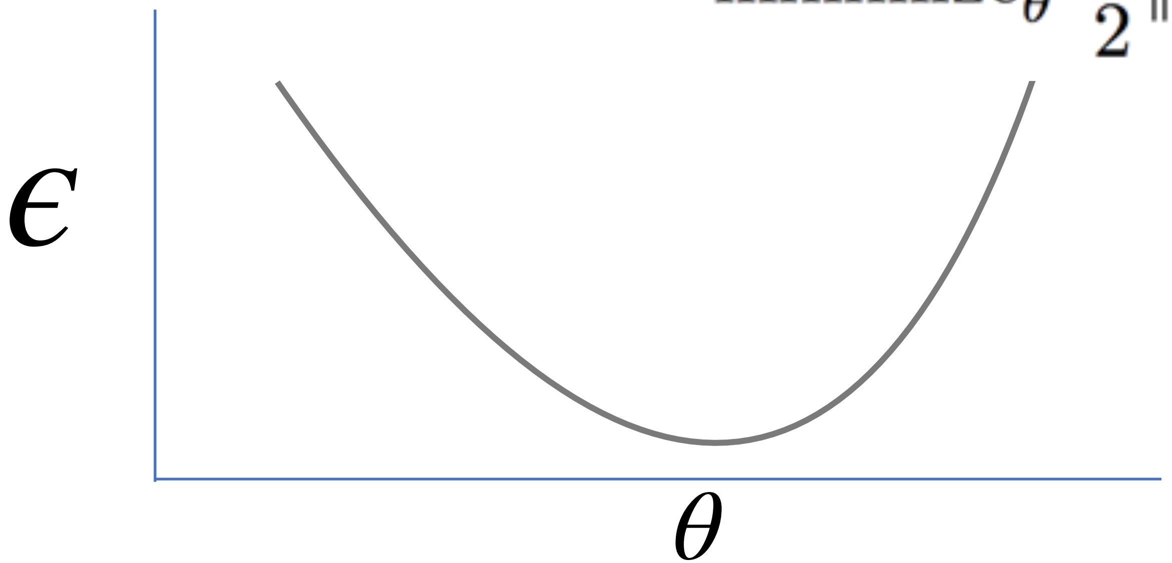
$$\text{minimize}_\theta \ \frac{1}{2}\|X\theta - y\|_2^2$$

$$\implies \text{minimize} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \epsilon_i^2$$

*Recall $||z||_2^2 = z^T z = \sum z_i^2$

ERROR FUNCTION

$$\text{minimize}_\theta \ \frac{1}{2}\|X\theta - y\|_2^2$$



$$\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \epsilon_i^2$$

GRADIENTS

Minimizing a multivariate function involves finding a point where the gradient is zero:

$$\nabla_\theta f(\theta) = 0 \text{ (the vector of zeros)}$$

Points where the gradient is zero are local minima

- If the function is convex, also a global minimum

Let's solve the least squares problem!

We'll use the multivariate generalizations of some concepts from MATH141/142 …

- Chain rule: $\nabla_\theta f(X\theta) = X^T \nabla_{X\theta} f(X\theta)$
- Gradient of squared ℓ^2 norm: $\nabla_\theta \|\theta - z\|_2^2 = 2(\theta - z)$

LEAST SQUARES

Recall the least squares optimization problem:

$$\text{minimize}_\theta \ \frac{1}{2}\|X\theta - y\|_2^2$$

What is the gradient of the optimization objective ????????

$$\nabla_\theta \frac{1}{2}\|X\theta - y\|_2^2 =$$

Chain rule:
$\nabla_\theta f(X\theta) = X^T \nabla_{X\theta} f(X\theta)$

$$X^T \nabla_{X\theta} \frac{1}{2}\|X\theta - y\|_2^2 =$$

Gradient of norm:
$\nabla_\theta \|\theta - z\|_2^2 = 2(\theta - z)$

$$\nabla_\theta \frac{1}{2}\|X\theta - y\|_2^2 = X^T(X\theta - y)$$

LEAST SQUARES

Recall: points where the gradient equals zero are minima.

$$\nabla_\theta \frac{1}{2}\|X\theta - y\|_2^2 = X^T(X\theta - y)$$

So where do we go from here?????????

Solve for model parameters θ

$$X^T(X\theta - y) = 0$$

$$X^T X\theta - X^T y = 0 \Rightarrow X^T X\theta = X^T y$$

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

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

LINEAR REGRESSION AS OPTIMIZATION PROBLEM

Let's consider linear regression that minimizes the sum of squared error, i.e., least squares …

1. **Hypothesis function: ????????**
    - Linear hypothesis function $h_\theta(x) = \theta^T x$

2. **Loss function: ????????**
    - Squared error loss $\ell(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$

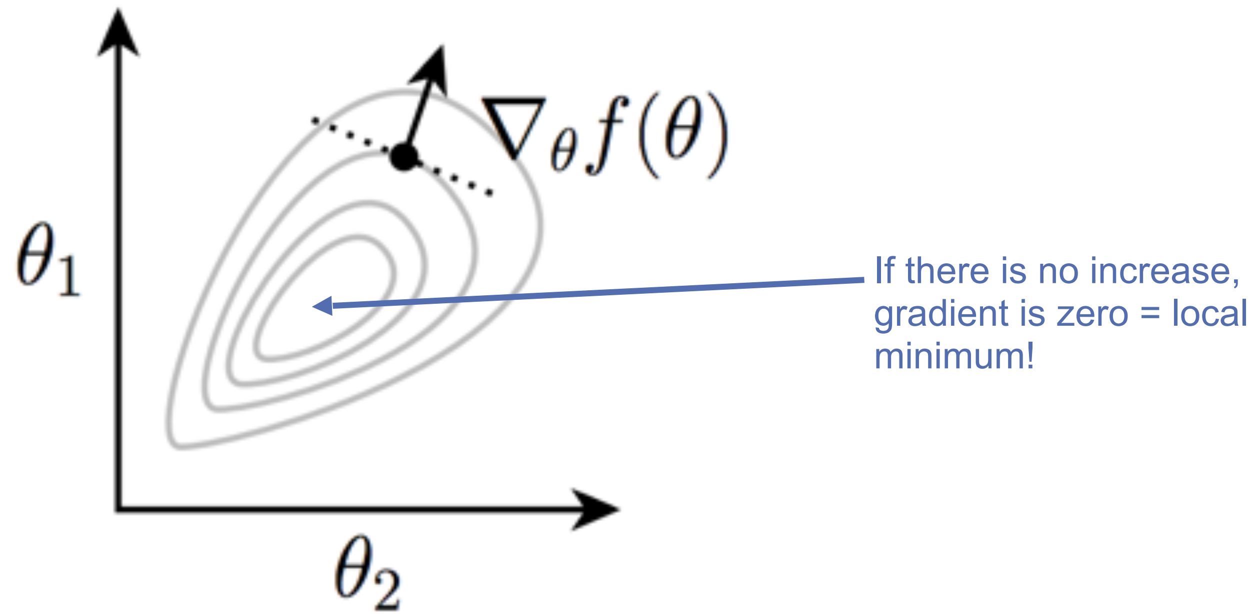
4. **Optimization problem: ????????**

$$\min_{\theta} \sum_{i=1}^{n} (\theta^T x^{(i)} - y^{(i)})^2$$

GRADIENT DESCENT

We used the gradient as a condition for optimality

It also gives the local direction of steepest increase for a function:



Intuitive idea: take small steps against the gradient.

Image from Zico Kolter

GRADIENT DESCENT

Algorithm for any* hypothesis function $h_\theta : \mathbb{R}^n \to \mathcal{Y}$, loss function $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_+$, step size α :

Initialize the parameter vector:

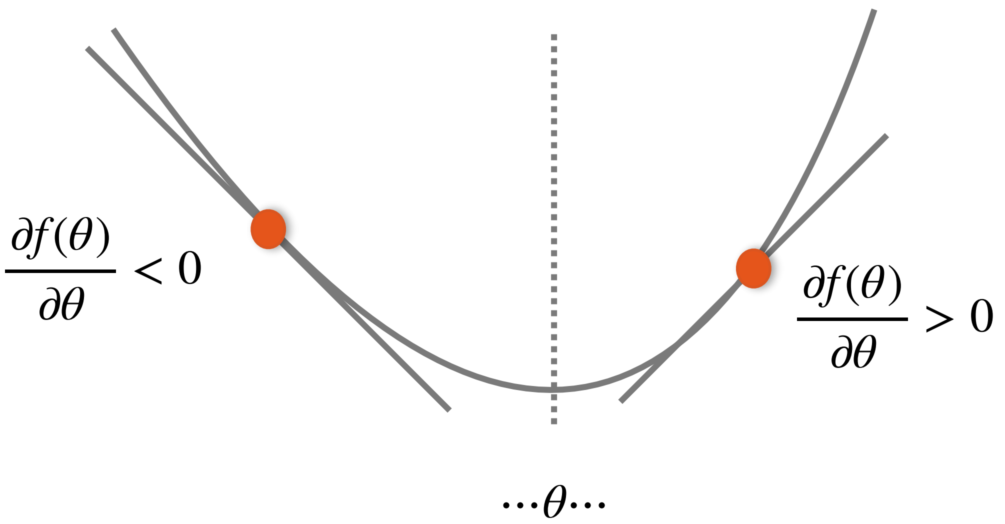
- $\theta \leftarrow 0$

Repeat until satisfied (e.g., exact or approximate convergence):

- **Compute gradient:** $g \leftarrow \sum_{i=1}^{n} \nabla_\theta \ell(h_\theta(x^{(i)}), y^{(i)})$
- **Update parameters:** $\theta \leftarrow \theta - \alpha \cdot g$

*must be reasonably well behaved

GRADIENT DESCENT



$$\theta := \theta - \alpha \frac{\partial f(\theta)}{\partial \theta}$$

EXAMPLE

Function: f(x,y) = $x^2 + 2y^2$

Gradient: ??????????

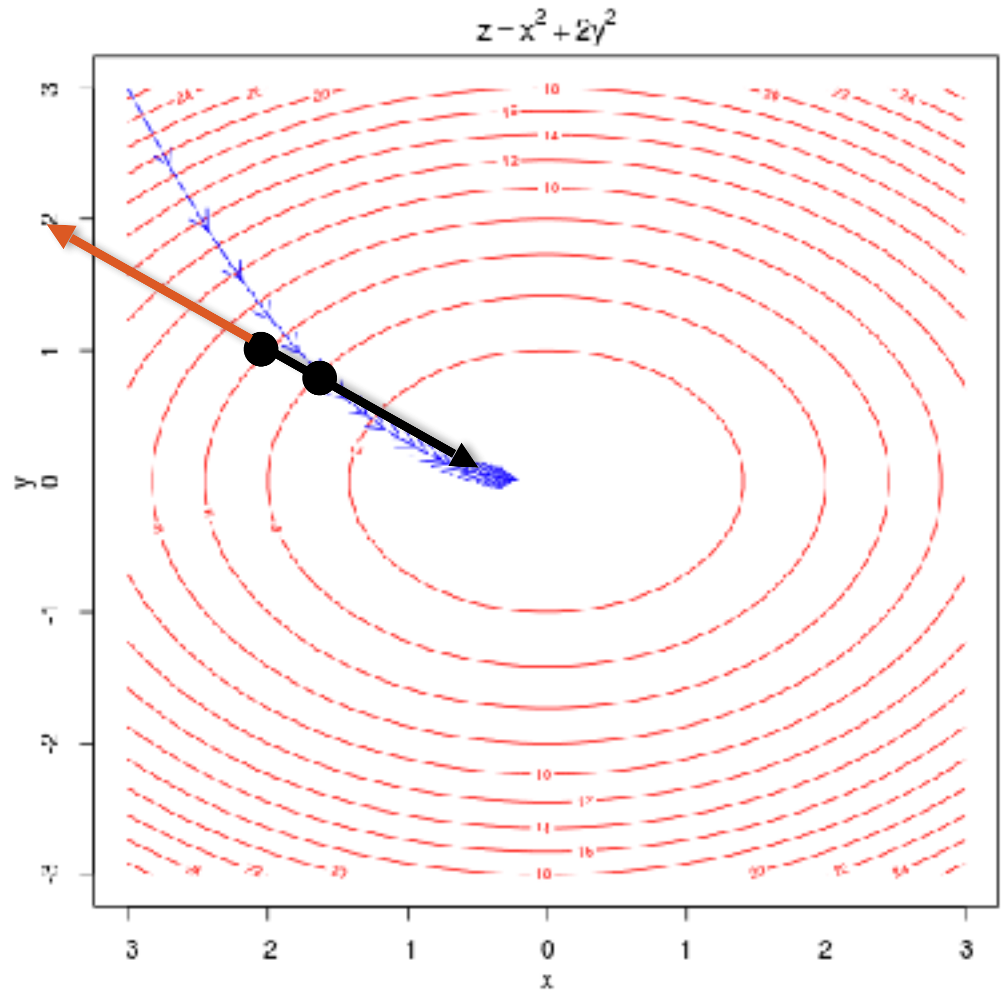
$$\nabla f(x, y) = \begin{bmatrix} 2x \\ 4y \end{bmatrix}$$

Let's take a gradient step from (-2, +1):

$$\nabla f(-2,1) = \begin{bmatrix} -4 \\ 1 \end{bmatrix}$$

Step in the direction (0.04, -0.01), scaled by step size

Repeat until no movement



GRADIENT DESCENT

$$\hat{y} = \theta_0 + \theta_1 x$$

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$$\theta_0 = 0.1 \qquad \theta_1 = 0.1$$

GRADIENT DESCENT

$$\hat{y} = \theta_0 + \theta_1 x$$

$\theta_0 = 0.1 \quad \theta_1 = 0.1$

x	y
0.2	0.44
0.31	0.123
0.45	0.75
0.26	0.39

GRADIENT DESCENT

$$\hat{y} = \theta_0 + \theta_1 x$$

$$\theta_0 = 0.1 \quad \theta_1 = 0.1$$

x	y	$\hat{y} = \theta_0 + \theta_1 x$
0.2	0.44	0.12
0.31	0.123	0.131
0.45	0.75	0.145
0.26	0.39	0.175

GRADIENT DESCENT

$$\hat{y} = \theta_0 + \theta_1 x$$

$\theta_0 = 0.1 \quad \theta_1 = 0.1$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$
0.2	0.44	0.12	0.0512
0.31	0.123	0.131	0.000032
0.45	0.75	0.145	0.183
0.26	0.39	0.175	0.0231

GRADIENT DESCENT

$\hat{y} = \theta_0 + \theta_1 x$

$\theta_0 = 0.1 \qquad \theta_1 = 0.1$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial(SSE)}{\partial\theta_0}$ $\hat{y} - y$
0.2	0.44	0.12	0.0512	-0.32
0.31	0.123	0.131	0.000032	0.008
0.45	0.75	0.145	0.183	-0.605
0.26	0.39	0.175	0.0231	-0.215

GRADIENT DESCENT

$\hat{y} = \theta_0 + \theta_1 x$

$\theta_0 = 0.1 \quad \theta_1 = 0.1$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial(SSE)}{\partial\theta_0}$ $\hat{y} - y$	$\frac{\partial(SSE)}{\partial\theta_1}$ $(\hat{y} - y)x$
0.2	0.44	0.12	0.0512	-0.32	-0.064
0.31	0.123	0.131	0.000032	0.008	0.00248
0.45	0.75	0.145	0.183	-0.605	-0.27225
0.26	0.39	0.175	0.0231	-0.215	-0.16125

GRADIENT DESCENT

$\hat{y} = \theta_0 + \theta_1 x$

$\theta_0 = 0.1 \quad \theta_1 = 0.1$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial(SSE)}{\partial\theta_0}$ $\hat{y} - y$	$\frac{\partial(SSE)}{\partial\theta_1}$ $(\hat{y} - y)x$
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0.26	0.39	0.175	0.0231	-0.215	-0.16125
				-1.132	-0.495

GRADIENT DESCENT

$\hat{y} = \theta_0 + \theta_1 x$

$\theta_0 = 0.1 \quad \theta_1 = 0.1$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial(SSE)}{\partial\theta_0}$ $\hat{y} - y$	$\frac{\partial(SSE)}{\partial\theta_1}$ $(\hat{y} - y)x$
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0.31	0.123	0.131	0.000032	0.008	0.00248
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				-1.132	-0.495

$$\theta_0 := \theta_0 - \alpha \sum_{i=1}^{n} \frac{\partial(SSE)}{\partial\theta_0} \qquad \theta_1 := \theta_1 - \alpha \sum_{i=1}^{n} \frac{\partial(SSE)}{\partial\theta_1}$$

GRADIENT DESCENT

$$\hat{y} = \theta_0 + \theta_1 x$$

$$\theta_0 = 0.1 \qquad \theta_1 = 0.1$$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial(SSE)}{\partial\theta_0}$ $\hat{y} - y$	$\frac{\partial(SSE)}{\partial\theta_1}$ $(\hat{y} - y)x$
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GRADIENT DESCENT

$\hat{y} = \theta_0 + \theta_1 x$

$\theta_0 = 0.1 \quad \theta_1 = 0.1$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial(SSE)}{\partial\theta_0}$ $\hat{y} - y$	$\frac{\partial(SSE)}{\partial\theta_1}$ $(\hat{y} - y)x$
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$$\theta_0 = 0.1 - 0.01 \times (-1.132)$$

GRADIENT DESCENT

$\hat{y} = \theta_0 + \theta_1 x$

$\theta_0 = 0.1 \quad \theta_1 = 0.1$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial(SSE)}{\partial\theta_0}$ $\hat{y} - y$	$\frac{\partial(SSE)}{\partial\theta_1}$ $(\hat{y} - y)x$
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$$\theta_0 = 0.1 - 0.01 \times (-1.132)$$

$$\theta_0 = 0.11132$$

GRADIENT DESCENT

$\hat{y} = \theta_0 + \theta_1 x$

$\theta_0 = 0.1 \quad \theta_1 = 0.1$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial(SSE)}{\partial\theta_0}$ $\hat{y} - y$	$\frac{\partial(SSE)}{\partial\theta_1}$ $(\hat{y} - y)x$
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$$\theta_0 := \theta_0 - \alpha \sum_{i=1}^{n} \frac{\partial(SSE)}{\partial\theta_0} \qquad \theta_1 := \theta_1 - \alpha \sum_{i=1}^{n} \frac{\partial(SSE)}{\partial\theta_1} \qquad \alpha = 0.01$$

$$\theta_0 = 0.1 - 0.01 \times (-1.132) \qquad \theta_1 = 0.1 - 0.01 \times (-0.495)$$

$$\theta_0 = 0.11132 \qquad \theta_1 = 0.10495$$

GRADIENT DESCENT

Algorithm for any* hypothesis function $h_\theta : \mathbb{R}^n \rightarrow \mathcal{Y}$, loss function $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$, step size α :

Initialize the parameter vector:

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Repeat until satisfied (e.g., exact or approximate convergence):

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- Update parameters: $\theta \leftarrow \theta - \alpha \cdot g$

$$\theta_0 := \theta_0 - \alpha \sum_{i=1}^{m} \frac{\partial(SSE)}{\partial \theta_0} \qquad \theta_1 := \theta_1 - \alpha \sum_{i=1}^{m} \frac{\partial(SSE)}{\partial \theta_1}$$

*must be reasonably well behaved

GRADIENT DESCENT - MULTIVARIATE

$$\theta \leftarrow \theta - \alpha \cdot g$$

$$\theta_0 := \theta_0 - \alpha \sum_{i=1}^{n} \frac{\partial(SSE)}{\partial \theta_0}$$

$$\theta_1 := \theta_1 - \alpha \sum_{i=1}^{n} \frac{\partial(SSE)}{\partial \theta_1}$$

$$\theta_2 := \theta_2 - \alpha \sum_{i=1}^{n} \frac{\partial(SSE)}{\partial \theta_2}$$

$$\vdots$$

$$\theta_m := \theta_n - \alpha \sum_{i=1}^{n} \frac{\partial(SSE)}{\partial \theta_m}$$

GRADIENT DESCENT - MULTIVARIATE

$$\frac{1}{n}\sum_{i=1}^{n}(h(\theta(x_i) - y_i)x_{ji} = \frac{\partial}{\partial\theta_j}f(\theta)$$

$\theta = 0$

Repeat{

obtain all partial derivatives w.r.t θ's first

$$\theta_j := \theta_j - \alpha\frac{1}{n}\sum_{i=1}^{n}(h(\theta(x_i) - y_i)x_{ji}$$

(update θ_j for all $j = 1 \ldots m$ simultaneously

}

$$\theta_0 := \theta_0 - \alpha\frac{1}{n}\sum_{i=1}^{n}(h(\theta(x_i) - y_i)x_{0i}$$

$$\theta_1 := \theta_1 - \alpha\frac{1}{n}\sum_{i=1}^{n}(h(\theta(x_i) - y_i)x_{1i}$$

$$\theta_2 := \theta_2 - \alpha\frac{1}{n}\sum_{i=1}^{n}(h(\theta(x_i) - y_i)x_{2i}$$

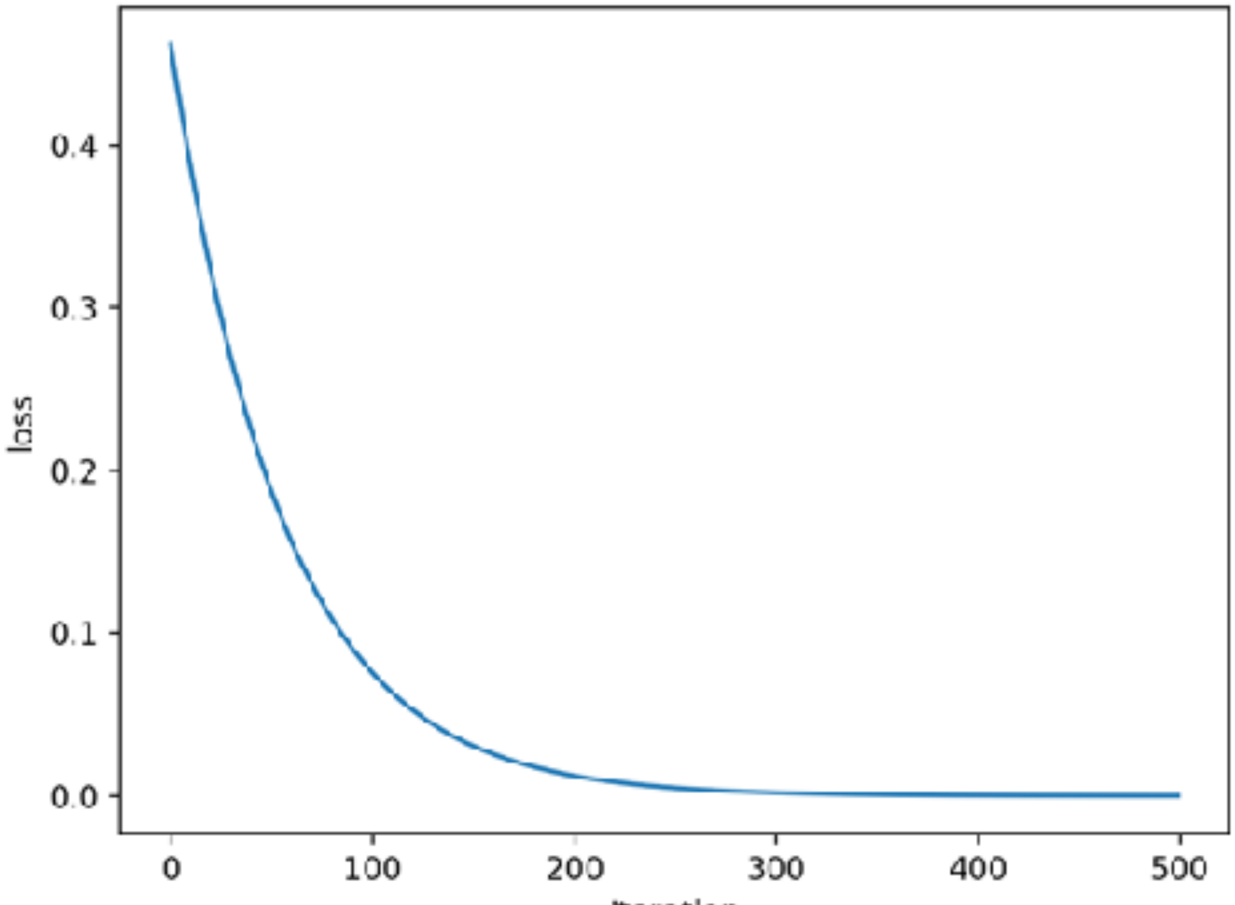
•

•

•

$$\theta_m := \theta_m - \alpha\frac{1}{n}\sum_{i=1}^{n}(h(\theta(x_i) - y_i)x_{mi}$$

PLOTTING LOSS OVER TIME



STOCHASTIC GRADIENT DESCENT - MULTIVARIATE

$$\frac{1}{n}\sum_{i=1}^{n}(h(\theta(x_i)-y_i)x_{ji} = \frac{\partial}{\partial\theta_j}f(\theta)$$

$\theta = 0$

Repeat{

obtain all partial derivatives w.r.t θ's first

$$\theta_j := \theta_j - \alpha\frac{1}{n}\sum_{i=1}^{n}(h(\theta(x_i)-y_i)x_{ji}$$

(update θ_j for all $j = 1 \ldots m$ simultaneously

}

STOCHASTIC GRADIENT DESCENT

$\theta = 0$

Repeat{

i = random index between 1 and m

$$\theta_j := \theta_j - \alpha(h(\theta(x_i)-y_i)x_{ji}$$

(update θ_j for all $j = 1 \ldots n$

}

GRADIENT DESCENT

$\hat{y} = \theta_0 + \theta_1 x$

$\theta_0 = 0.1 \quad \theta_1 = 0.1$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial(SSE)}{\partial\theta_0}$ $\hat{y} - y$	$\frac{\partial(SSE)}{\partial\theta_1}$ $(\hat{y} - y)x$
0.2	0.44	0.12	0.0512	-0.32	-0.064
0.31	0.123	0.131	0.000032	0.008	0.00248
0.45	0.75	0.145	0.183	-0.605	-0.27225
0.26	0.39	0.175	0.0231	-0.215	-0.16125
				-1.132	-0.495

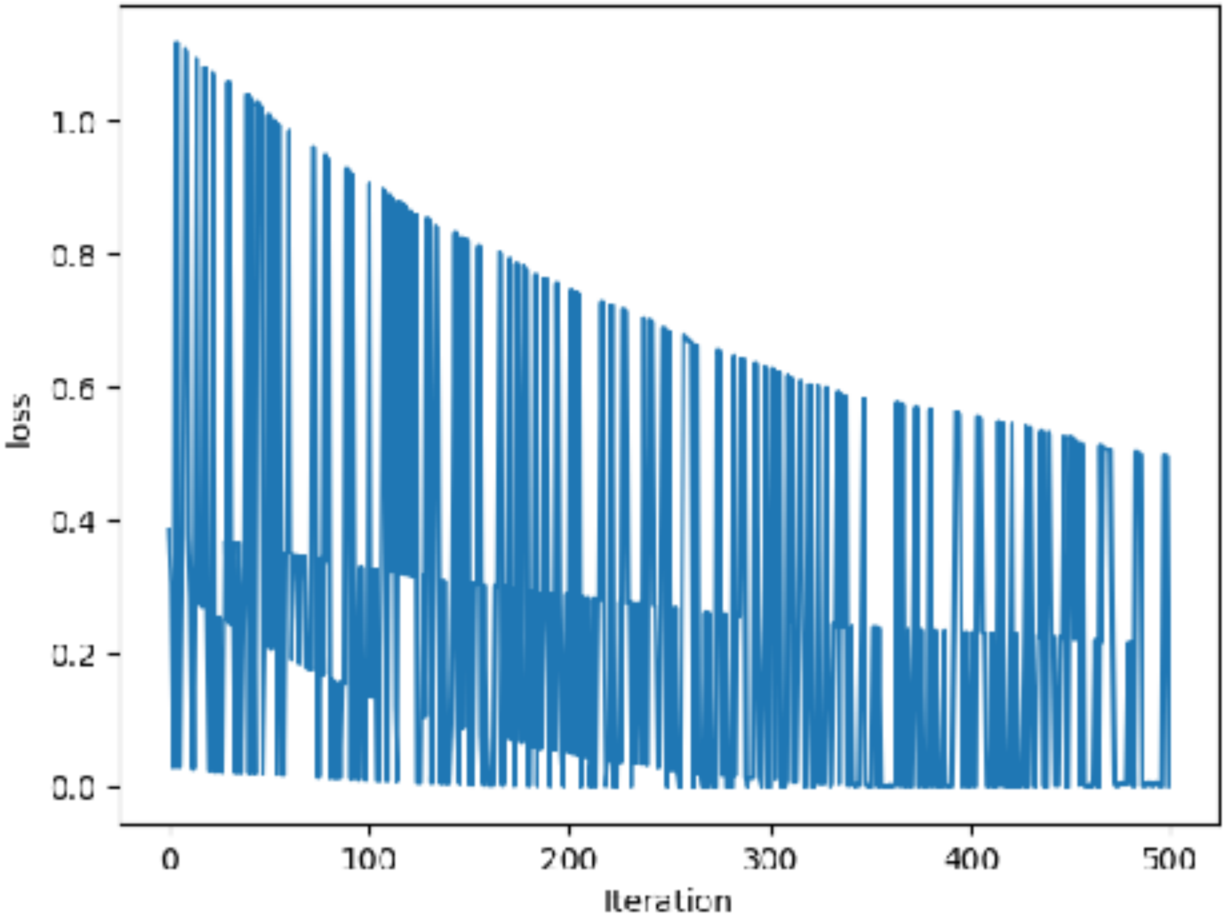
GRADIENT DESCENT

$\hat{y} = \theta_0 + \theta_1 x$

$\theta_0 = 0.1 \quad \theta_1 = 0.1$

x	y	$\hat{y} = \theta_0 + \theta_1 x$	SSE $\frac{1}{2}(\hat{y} - y)^2$	$\frac{\partial(SSE)}{\partial\theta_0}$ $\hat{y} - y$	$\frac{\partial(SSE)}{\partial\theta_1}$ $(\hat{y} - y)x$	……..
0.31	0.123	0.131	0.000032	0.008	0.00248	

STOCHASTIC GRADIENT DESCENT



STOCHASTIC GRADIENT DESCENT - MINI BATCH

$\theta = 0$

Repeat {

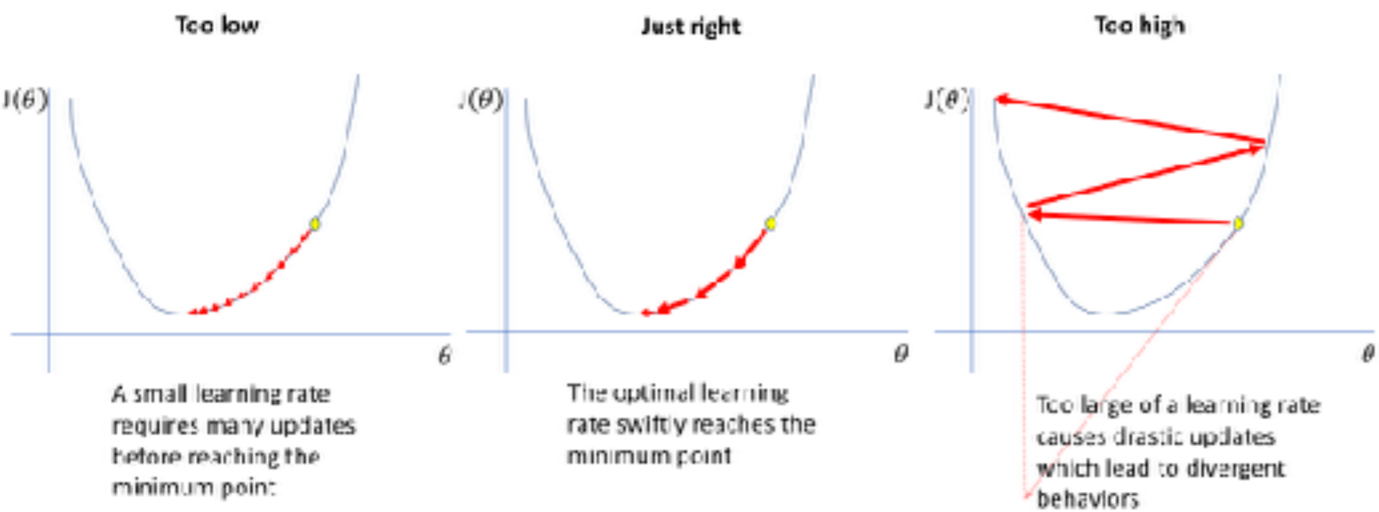
$i_1, \ldots, i_l$ = random index between 1 and m

$$\theta_j := \theta_j - \alpha \frac{1}{l} \sum_{i=1}^{l} (h(\theta(x_i) - y_i)x_{ji}$$

(update θ_j for all $j = 1 \ldots n$

}

Gradient Descent



GRADIENT DESCENT IN PURE(-ISH) PYTHON

```
# Training data (X, y), T time steps, alpha step
def grad_descent(X, y, T, alpha):
    m, n = X.shape           # m = #examples, n = #features
    theta = np.zeros(n)      # initialize parameters
    f = np.zeros(T)          # track loss over time
```

```
    for i in range(T):
        # loss for current parameter vector theta
        f[i] = 0.5*np.linalg.norm(X.dot(theta) – y)**2
        # compute steepest ascent at f(theta)
        g = np.transpose(X).dot(X.dot(theta) – y)
        # step down the gradient
        theta = theta – alpha*g
    return theta, f
```

Implicitly using squared loss and linear hypothesis function above; drop in your favorite gradient for kicks!