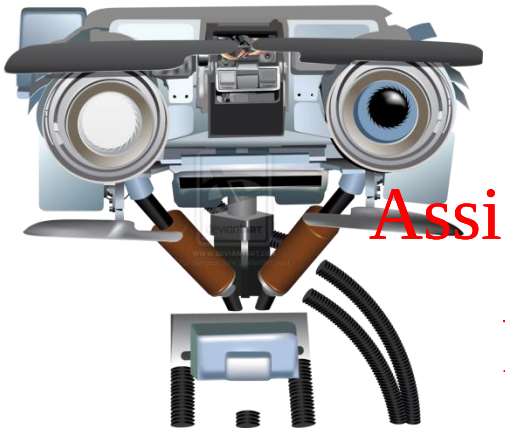


Supervised Learning I: Regression

Today

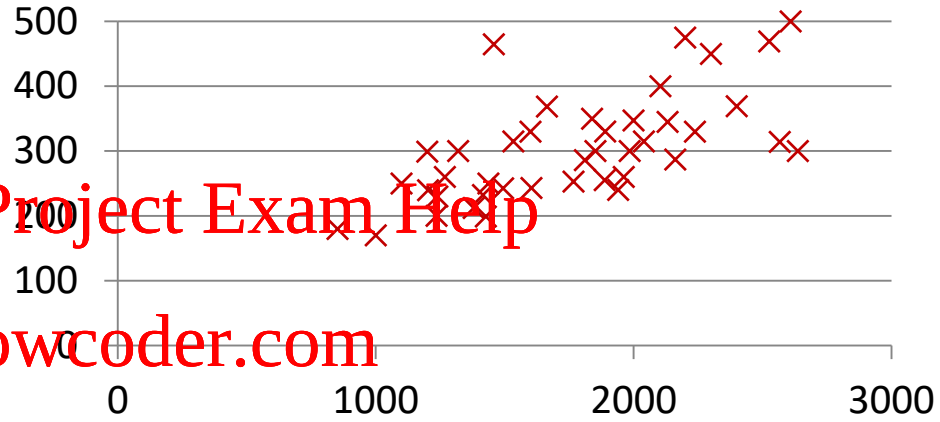
- Multivariate linear regression
- Solution for SSD cost
  - Indirect
  - Direct
- Maximum likelihood cost

Linear Regression

Hypothesis:

$$h_\theta(x) = \theta_0 + \theta_1 x$$

θ_i's: Parameters



Cost Function:

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$$

SSD = sum of squared differences, also
SSE = sum of squared errors

Multidimensional inputs

Size (feet^2)	Number of bedrooms	Number of floors	Age of home (years)	Price ($1000)
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
…	…	…	…	…

Notation:

n = number of features

$x^{(i)}$ = input (features) of i^{th} training example.

$x_j^{(i)}$ = value of feature j in i^{th} training example.

Multivariate Linear Regression

Hypothesis:

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

For convenience of notation, define $x_0 = 1$.

θ_i 's: Parameters

Cost Function:

$$J(\theta_0, \theta_1, \ldots, \theta_n) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

Goal: $\underset{\theta_0, \theta_1, \ldots, \theta_n}{\text{minimize}}\ J(\theta_0, \theta_1, \ldots, \theta_n)$ **How??**

Two potential solutions

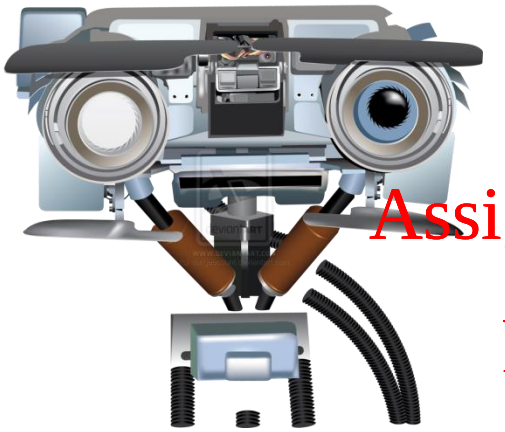
$$\min_{\theta} J(\theta; x^{(1)}, y^{(1)}, \ldots, x^{(m)}, y^{(m)})$$

Gradient descent (another iterative algorithm)

- Start with a guess for θ
- Change θ to decrease $J(\theta)$
- Until reach minimum

Direct minimization

- Take derivative, set to zero
- Sufficient condition for minima
- Not possible for most “interesting” cost functions



Solving Linear Regression

Gradient Descent

Gradient Descent Algorithm

Set $\theta = 0$

Repeat {

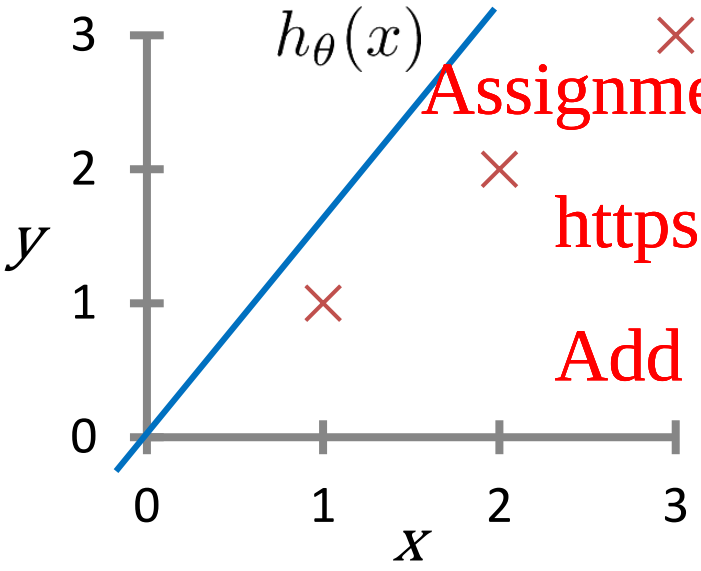
$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \qquad \text{simultaneously for all } j = 0, \ldots, n$$

} until convergence

Gradient Descent: Intuition

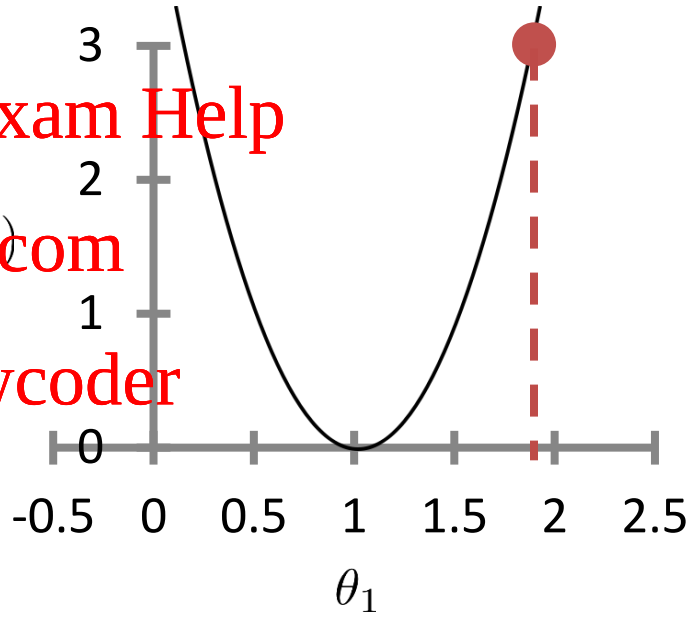
$h_\theta(x)$

(for fixed θ_1, this is a function of x)



$J(\theta_1)$

(function of the parameter θ_1)

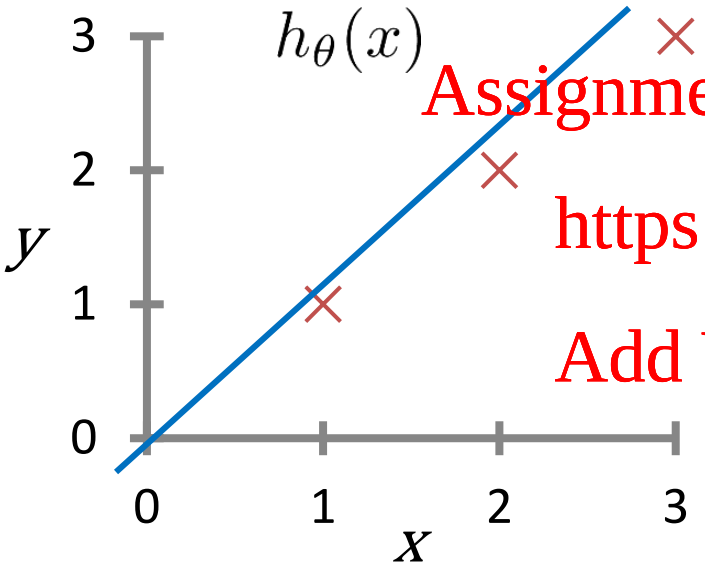


$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

Gradient Descent: Intuition

$h_\theta(x)$

(for fixed θ_1, this is a function of x)



$J(\theta_1)$

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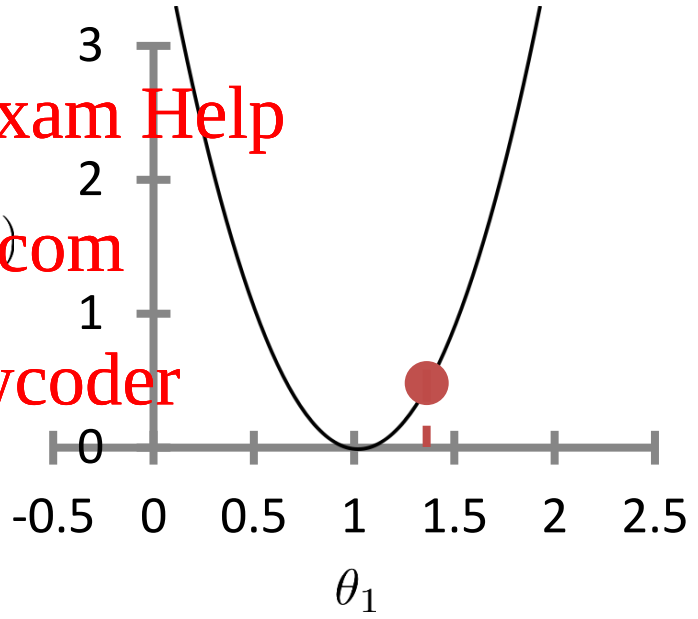
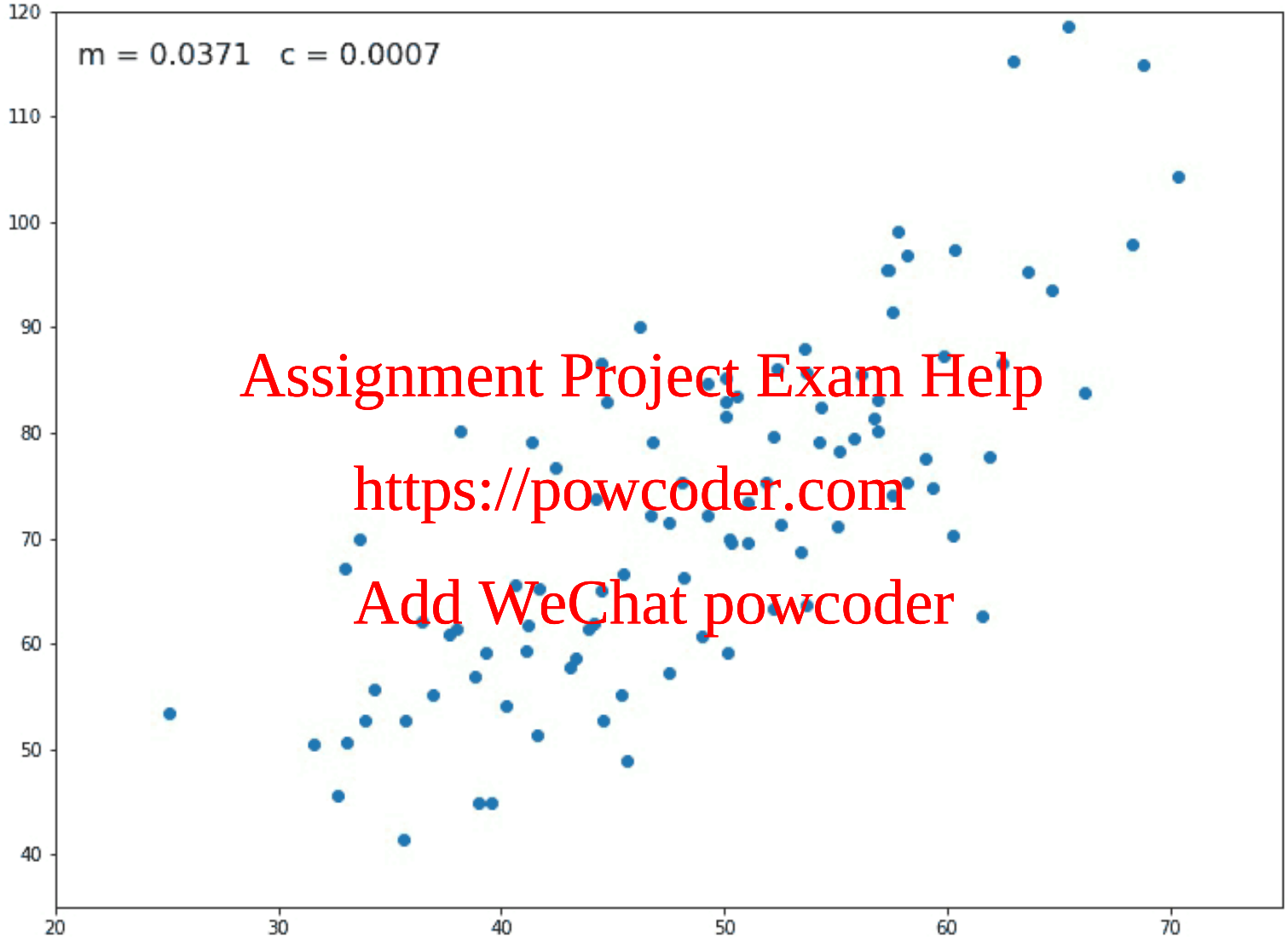


$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$



Gradient descent illustration (credit: https://towardsdatascience.com/

Gradient for Least Squares Cost

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

$$\frac{\partial}{\partial \theta_j} J(\theta) =$$

Gradient for Least Squares Cost

For one example

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \frac{1}{2} \left(h_\theta(x) - y \right)^2$$

Gradient for Least Squares Cost

For one example

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_\theta(x) - y)^2$$

$$= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} (h_\theta(x) - y)$$

Gradient for Least Squares Cost

For one example

$$\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_\theta(x) - y)^2 \\
&= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} (h_\theta(x) - y) \\
&= (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{n} \theta_i x_i - y \right)
\end{aligned}$$

Gradient for Least Squares Cost

For one example

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_\theta(x) - y)^2$$

$$= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} (h_\theta(x) - y)$$

$$= (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{n} \theta_i x_i - y \right)$$

$$= (h_\theta(x) - y)\, x_j$$

What is this?

Gradient Descent Algorithm

Set $\boldsymbol{\theta} = 0$

Repeat {

$$\boldsymbol{\theta}_j := \boldsymbol{\theta}_j - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta\left(\boldsymbol{x}^{(i)}\right) - y^{(i)} \right) \boldsymbol{x}_j^{(i)}$$

simultaneously for all $j = 0, \ldots, n$

} until convergence

in vector form?

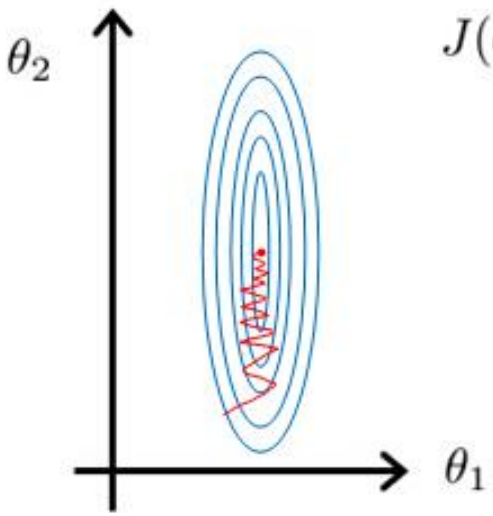
$$\boldsymbol{\theta} := \boldsymbol{\theta} + \alpha \frac{1}{m} \boldsymbol{e}^T \boldsymbol{X}$$

$$\boldsymbol{e}_i = h_\theta\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}$$

$$\boldsymbol{X} = \begin{bmatrix} x_1^{(1)} & \cdots & x_n^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(m)} & \cdots & x_n^{(m)} \end{bmatrix}$$

Feature normalization

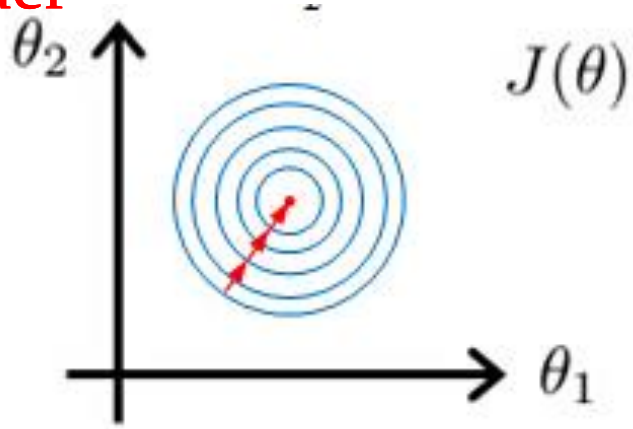
- If features have very different scale, GD can get "stuck" since x_j affects size of gradient in the direction of j[th] dimension
- Normalizing features to be zero-mean (μ) and same-variance (σ) helps gradient descent converge faster

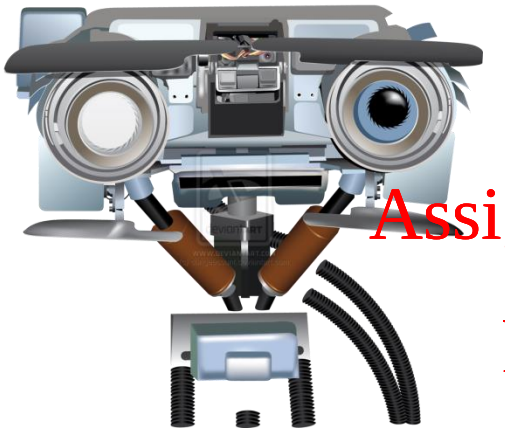


$J(\theta)$

normalize

$$x_j^{(i)} = \frac{x_j^{(i)} - \mu_j}{\sigma_j}$$





Solving Linear Regression

Direct Solution

Direct solution

Want to minimize SSD:

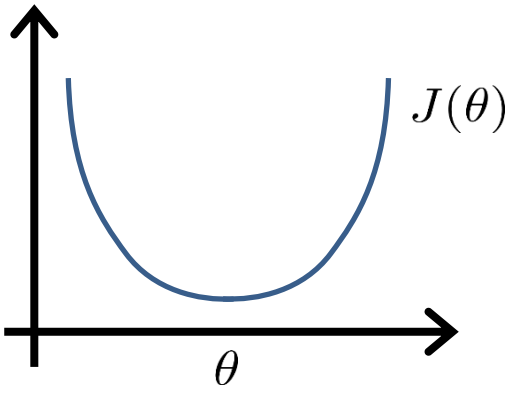
$$J(\theta_0, \theta_1, \ldots, \theta_m) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

Find minima of functions:

$\theta \in \mathbb{R}^{n+1}$

$\frac{\partial}{\partial \theta_j} J(\theta) = \cdots = 0$ (for every j)

Solve for $\theta_0, \theta_1, \ldots, \theta_n$



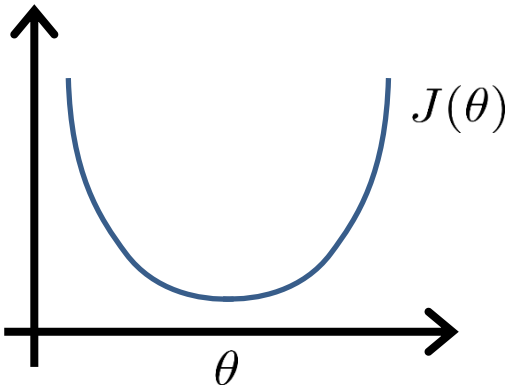
Direct solution

Re-write SSD using vector-matrix notation:

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

Where:

$$X = \begin{bmatrix} — (x^{(1)})^T — \\ — (x^{(2)})^T — \\ \vdots \\ — (x^{(m)})^T — \end{bmatrix} \quad y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$



Solution: Normal Equation

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

Derivation of Normal Equations

- SSE in matrix form:

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

$$= \frac{1}{2m}\{\theta^T\{X^T X\}\,\theta - 2\{X^T y\}^T\theta + const\}$$

- Take derivative with respect to θ (vector), set to 0

$$\frac{\partial J}{\partial \theta} \propto X^T X\,\theta - X^T y = 0$$ ignore constant multiplier

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

- Also known as the least mean squares, or least squares solution

Example: $m = 4.$

x_0	Size (feet²) x_1	Number of bedrooms x_2	Number of floors x_3	Age of home (years) x_4	Price ($1000) y
1	2104	5	1	45	460
1	1416	3	2	40	232
1	1534	3	2	30	315
1	852	2	1	36	178

Design Matrix

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \end{bmatrix} \qquad y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix}$$

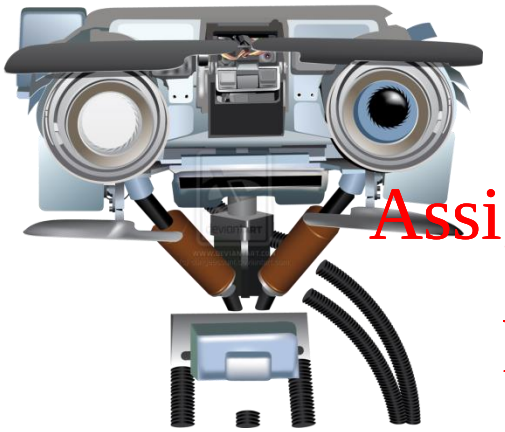
Normal Equation

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

Trade-offs

m training examples, *n* features.

Gradient Descent	Normal Equations
• Need to choose α. • Needs many iterations. • Works well even when *n* is large.	• No need to choose α. • Don't need to iterate. • Need to compute $(X^T X)^{-1}$ • Slow if *n* is very large.



Maximum Likelihood for Linear Regression

So far, we have treated outputs as noiseless

- Defined cost function as “distance to true output”

- An alternate view:

  - data (x,y) are generated by unknown process
  - however, we only observe a noisy version

  - how can we model this uncertainty?

- Alternative cost function?

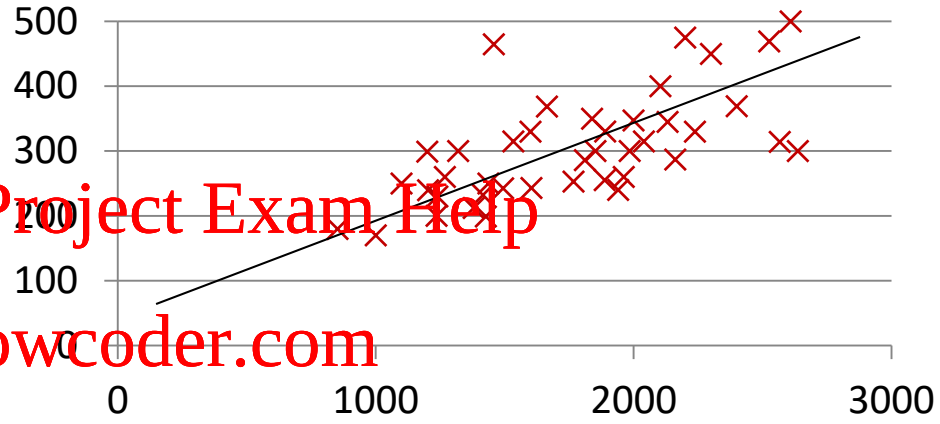
How to model uncertainty in data?

Hypothesis:

$h_\theta(x) = \theta^T x$

θ: parameters

$D = \left(x^{(i)}, y^{(i)}\right)$: data

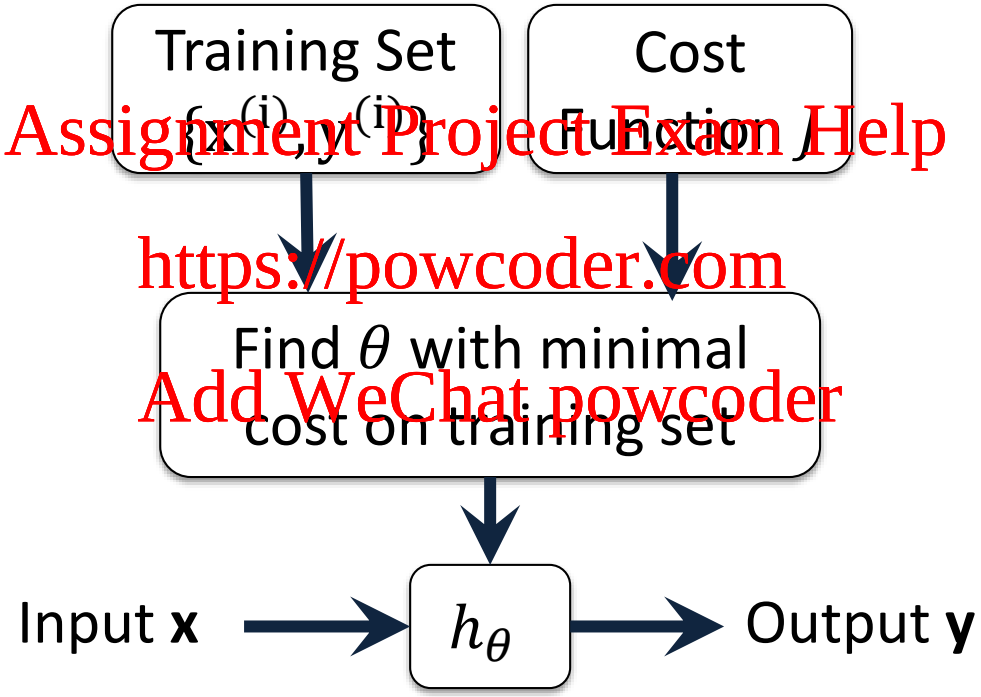


New cost function:

maximize probability of data given model:

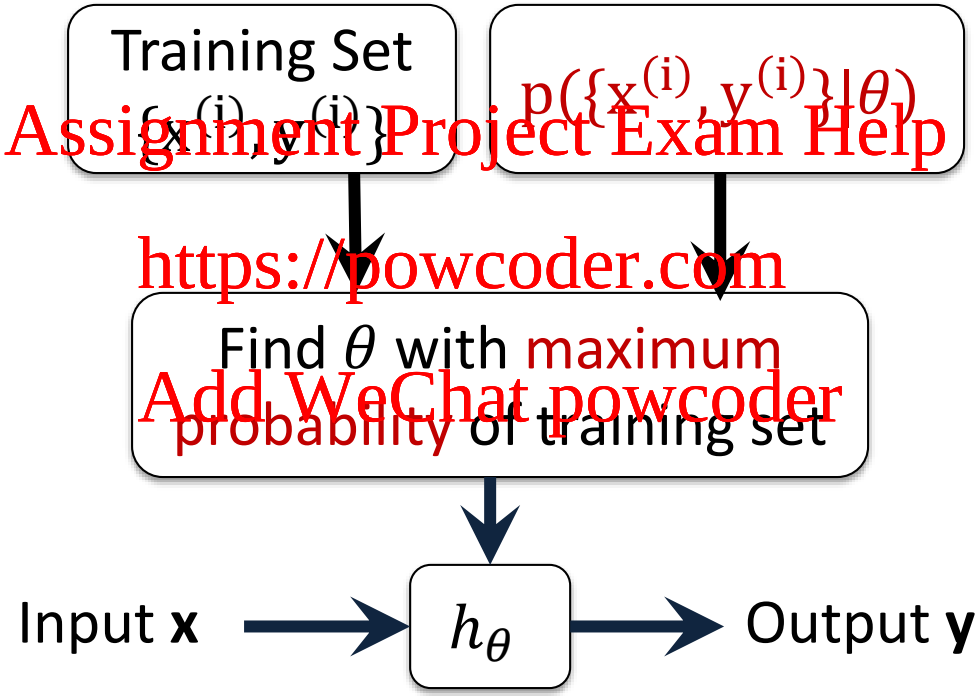
$$p((x^{(i)}, y^{(i)})|\theta)$$

Recall: Cost Function



Alternative View:

"Maximum Likelihood"



Maximum Likelihood: Example

- Intuitive example: Estimate a coin toss

  I have seen 3 flips of heads, 2 flips of tails, what is the chance of head (or tail) of my next flip?

- Model:

  Each flip is a Bernoulli random variable X

  X can take only two values: 1 (head), 0 (tail)

$$p(X = 1) = \theta, \quad p(X = 0) = 1 - \theta$$

- θ is a parameter to be identified from data

Maximum Likelihood: Example

- 5 (independent) trials

$X_1 = 1 \quad X_2 = 0 \quad X_3 = 1 \quad X_4 = 1 \quad X_5 = 0$

- Likelihood of all 5 observations:

$$p(X_1, \ldots, X_5|\theta) = \theta^3(1-\theta)^2$$

- Intuition

ML chooses θ such that likelihood is maximized

Maximum Likelihood: Example

- 5 (independent) trials


$X_1 = 1$


$X_2 = 0$


$X_3 = 1$


$X_4 = 1$


$X_5 = 0$

- Likelihood of all 5 observations:

$$p(X_1, \ldots, X_5|\theta) = \theta^3(1-\theta)^2$$

- Solution (left as exercise)

$$\theta_{ML} = \frac{3}{(3+2)}$$

i.e. fraction of heads in total number of trials

PSet 1 Out

- Due on Tuesday 9/15 11:59pm GMT -5 (Boston Time)
- Diagnostic homework covering topics covered in prereqs

Next Class

Supervised Learning II: Classification:

classification; sigmoid function; logistic regression.

Reading: Bishop 4.3.1-4.3.2; 4.3.4

overview of logistic regression