CS2109S: Introduction to AI and Machine Learning

Lecture 5: Linear Regression

15 September 2023

Admin

- **Midterm (Confirmed)**
  - Date & Time: **6 October, 10:00 – 12:00**
  - Venue: **MPSH 1A**
  - Notes:
    - Please come at 9:30. You are **allowed into hall at 9:45**
    - Materials: all topics covered before recess week **until Lecture 4**
    - Cheatsheet: 1 x A4 paper, both sides

Recap

- **Machine Learning**
  - What is ML? – machine that learns through data
  - Types of Feedback: supervised, unsupervised, semi-supervised, reinforcement
  - Supervised Learning
- **Performance Measure**
  - Regression: mean squared error, mean absolute error
  - Classification: correctness, accuracy, confusion matrix, precision, recall, F1
- **Decision Trees**
  - Decision Tree Learning (DTL): greedy, top-down, recursive algorithm
  - Entropy and Information Gain
  - Different types of attributes: many values, differing costs, missing values
  - Pruning: min-sample, max-depth
  - Ensemble Methods: bagging, boosting

ERRATA

Decision Tree Learning

with Information Gain

```
def DTL(examples, attributes, default):
    if examples is empty: return default
    if examples have the same classification:
        return classification
    if attributes is empty:
        return mode(examples)
    best = choose_attribute(attributes, examples)
    tree = a new decision tree with root best
    for each value v_i of best:
        examples_i = {rows in examples with best = v_i}
        subtree = DTL(examples_i, attributes – best, mode(examples))
        add a branch to tree with label v_i and subtree subtree
```

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	\$\$\$	F	T	French	0–10	T
X_2	T	F	F	T	Full	\$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	\$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	\$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	\$\$\$	F	T	French	>60	F
X_6	F	T	F	T	Some	\$\$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	\$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	\$\$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	\$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	\$\$\$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	\$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	\$	F	F	Burger	30–60	T

(2,4,6) (2,2,4,4)

Patrons: (2,4,6)

2 x F 4 x T 2 x T, 4 x F

$$IG(Patrons) = 1 - \left[\frac{2}{12} I(0,1) + \frac{4}{12} I(1,0) + \frac{6}{12} I\left(\frac{2}{6}, \frac{4}{6}\right)\right] = 0.541\ bits$$

Type: (2,2,4,4)

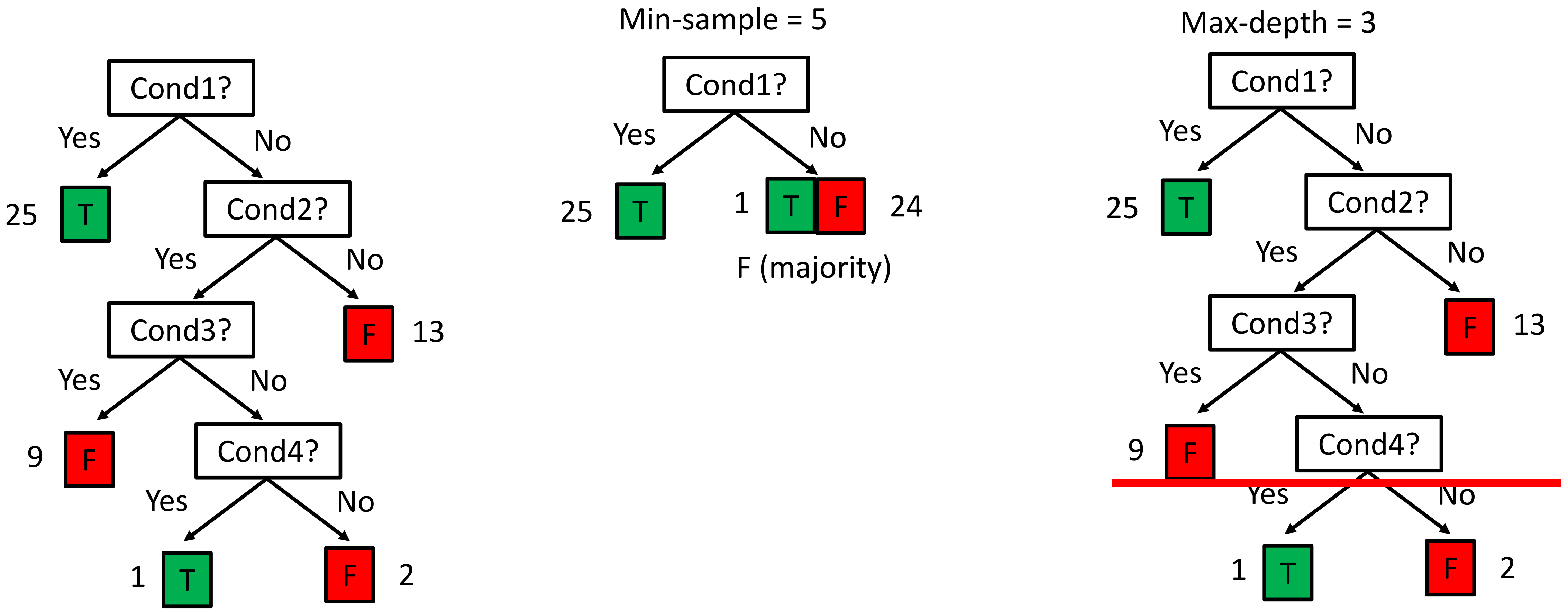
T+F T+F 2T, 2F 2T, 2 F

$$IG(Type) = 1 - [\frac{2}{12} I(\frac{1}{2}, \frac{1}{2}) + \frac{2}{12} I(\frac{1}{2}, \frac{1}{2}) + \frac{4}{12} I(\frac{2}{4}, \frac{2}{4}) + \frac{4}{12} I(\frac{2}{4}, \frac{2}{4})] = 0 \text{ bits}$$

ERRATA

Pruning

Prevent nodes from being split even when if fails to cleanly separate examples.



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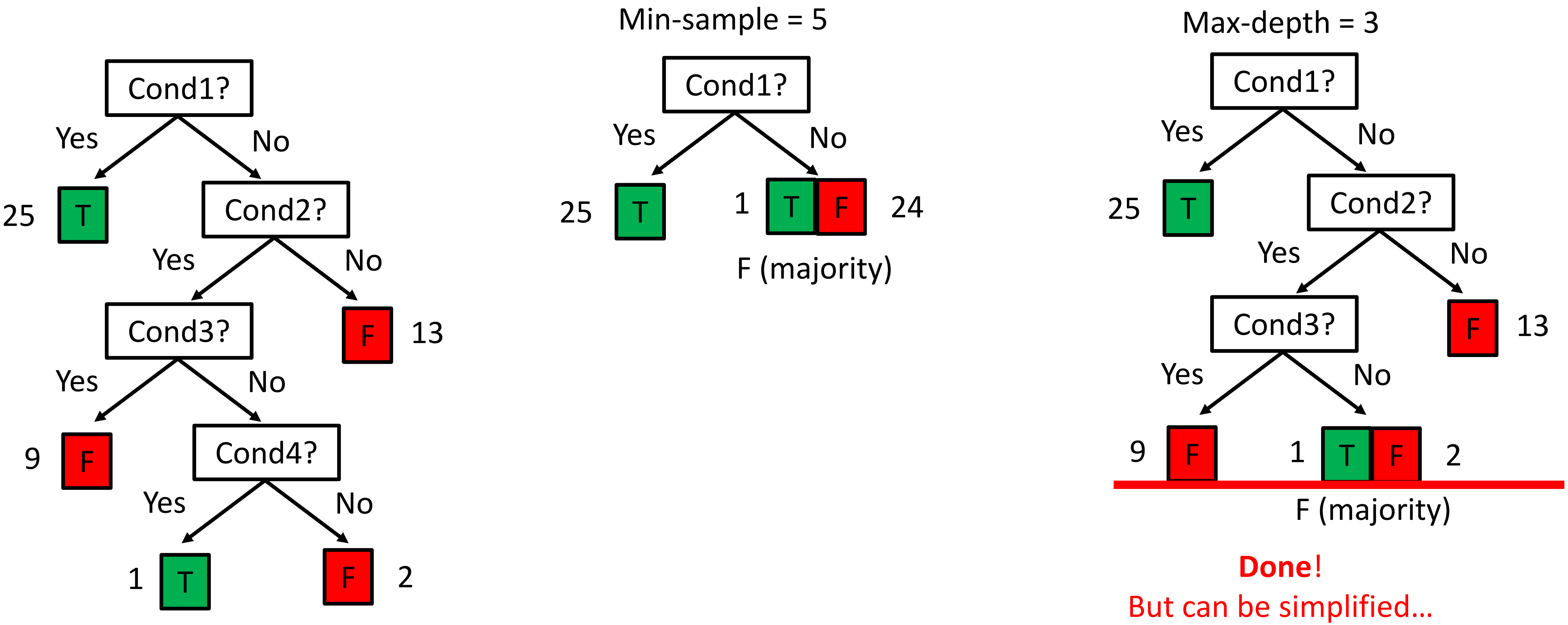

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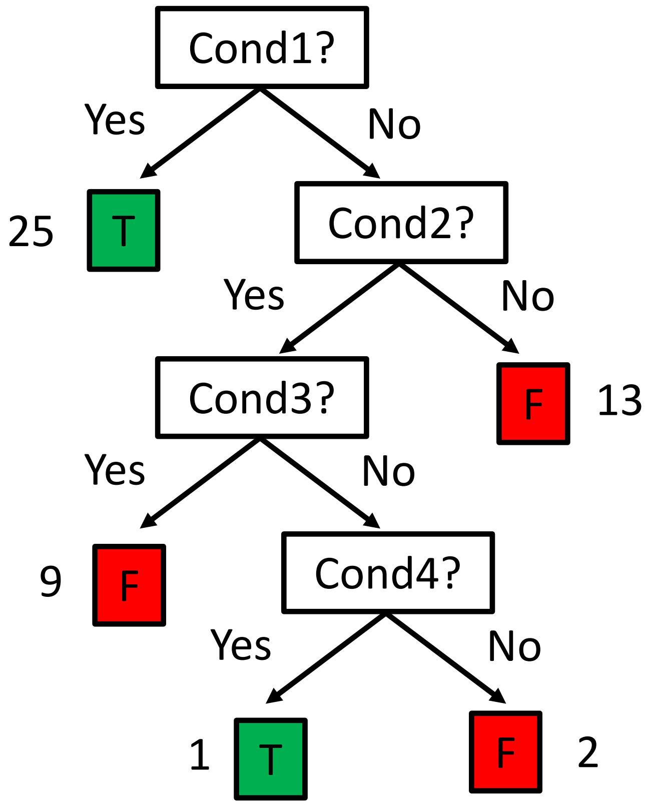

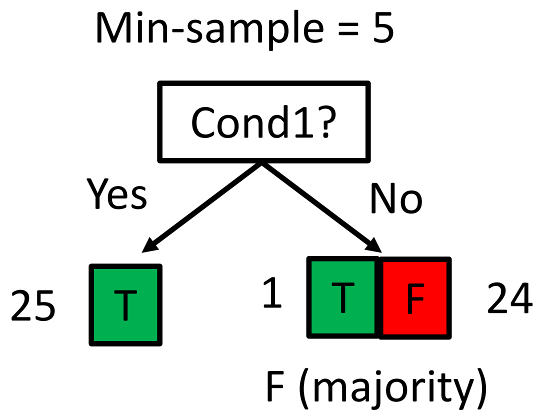

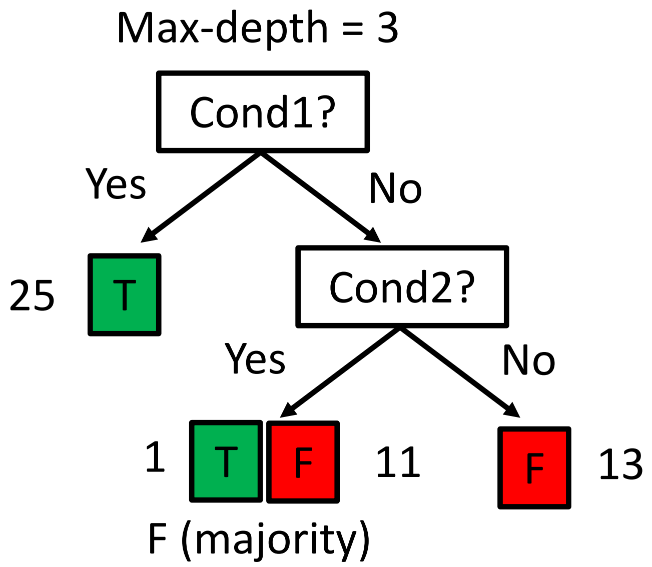

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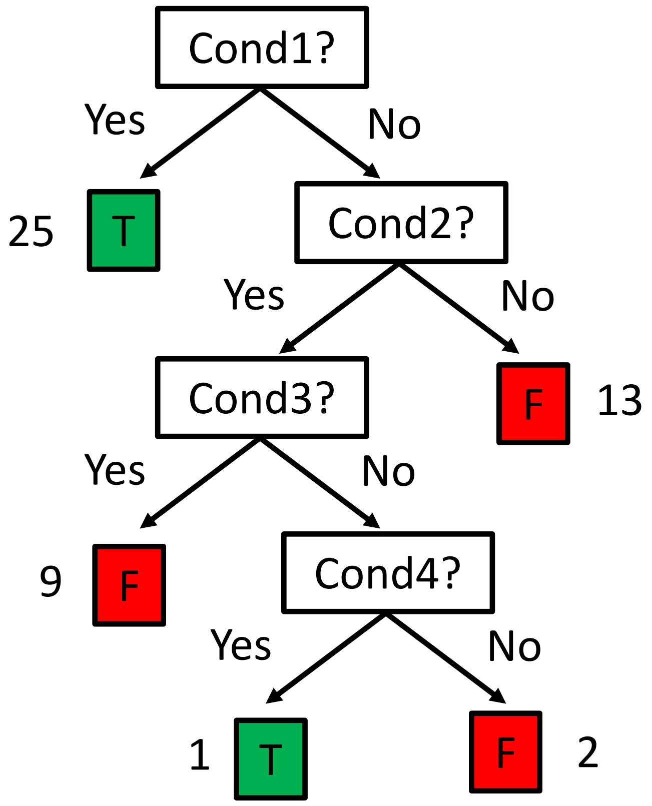
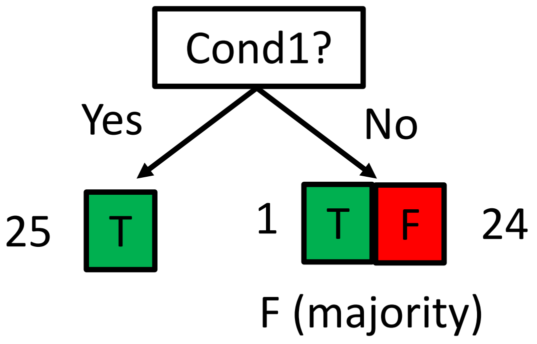
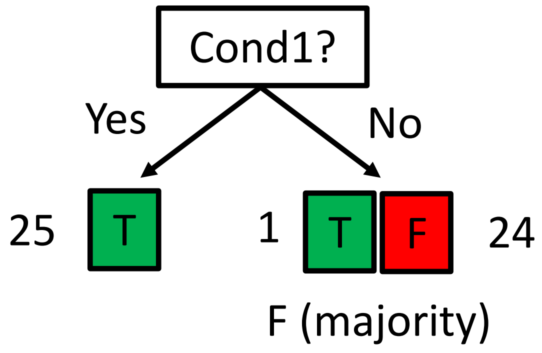


Min-sample = 5



Max-depth = 3



Outline

- Linear Regression
- Gradient Descent
  - Gradient Descent Algorithm
  - Linear Regression with Gradient Descent
  - Variants of Gradient Descent
- Linear Regression: Challenges and Solutions
  - Linear Regression with Many Attributes
  - Dealing with Features of Different Scales
  - Dealing with Non-Linear Relationship
- Normal Equation

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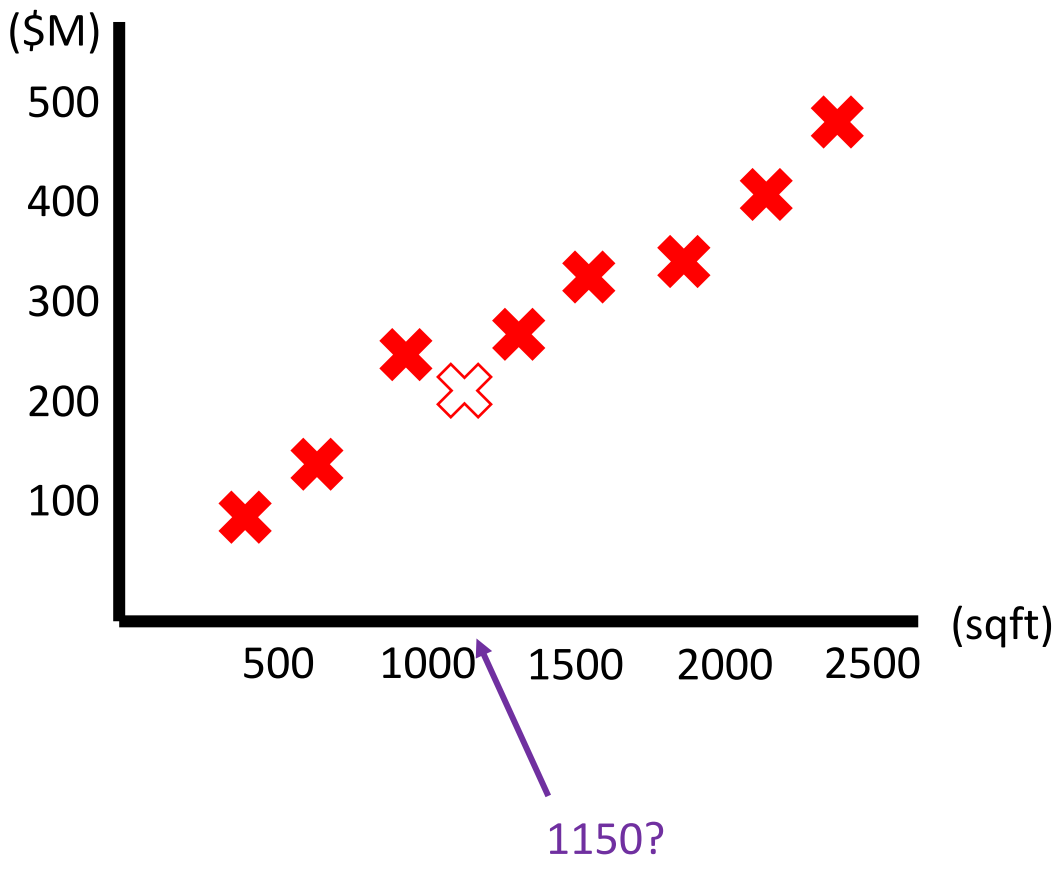
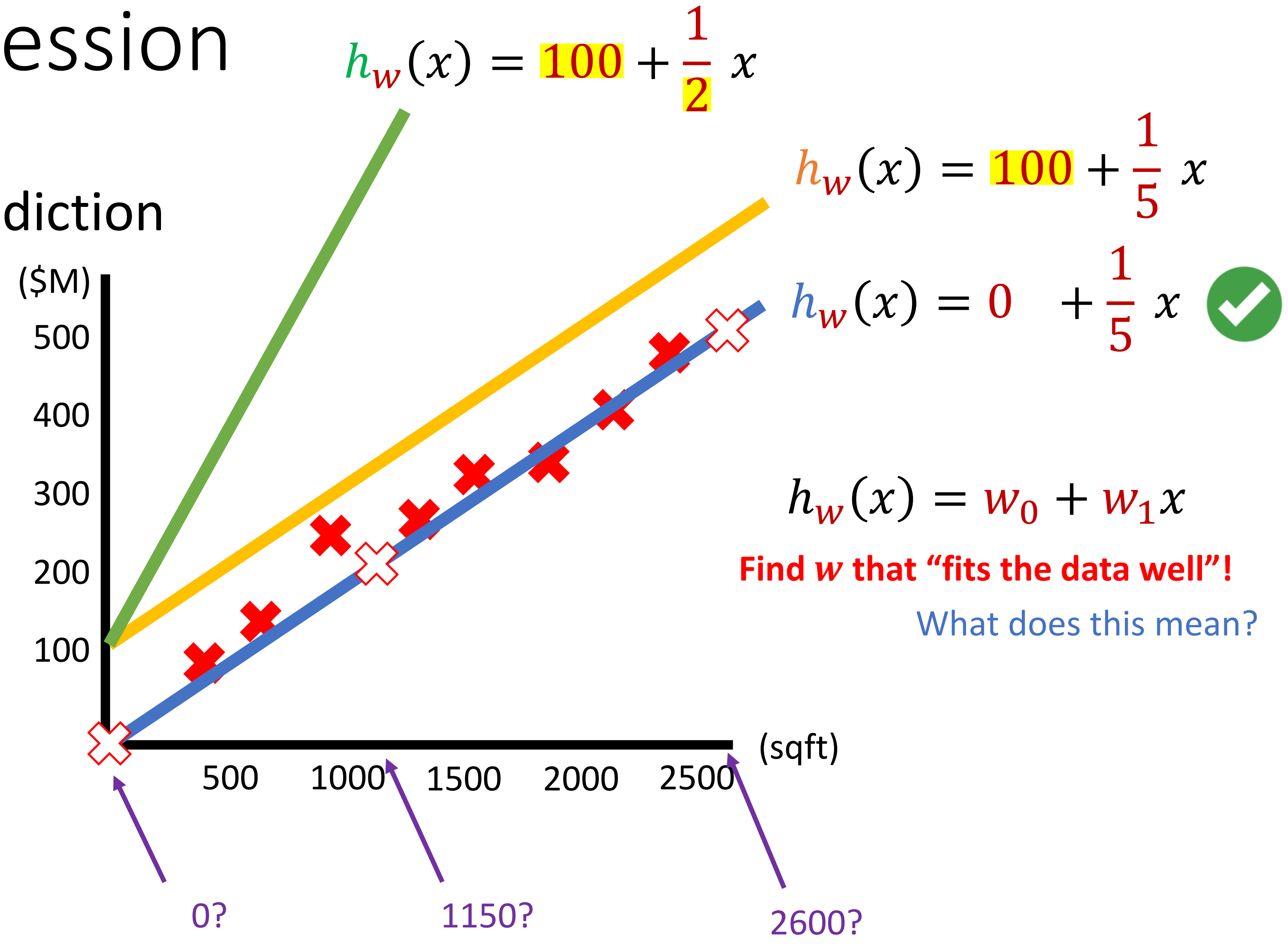
Regression

Housing price prediction



Linear Regression

Housing price prediction



$$h_w(x) = w_0 + w_1 x$$

Find w that "fits the data well"!

What does this mean?

Linear Regression: Measuring Fit

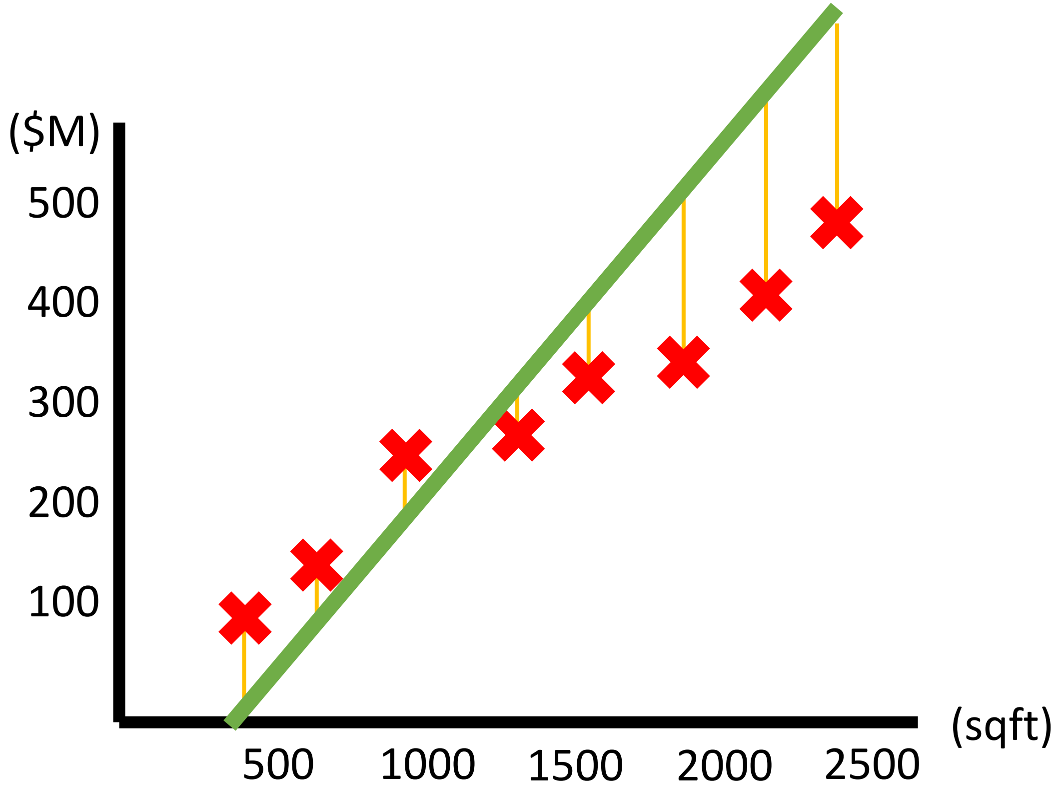
For a set of m examples
$\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$
we can compute the average (mean) **squared error** as follows.

$$J_{MSE}(w) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_w(x^{(i)}) - y^{(i)}\right)^2$$

Loss function

$\hat{y}^{(i)}$

Want to minimize the loss/error!

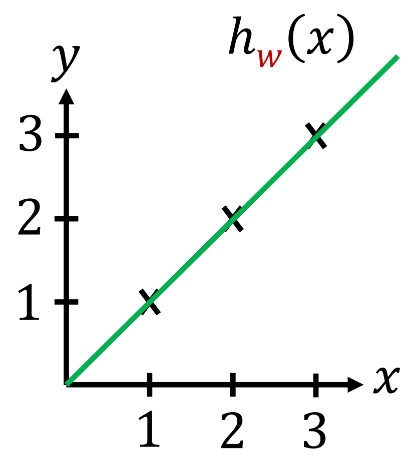


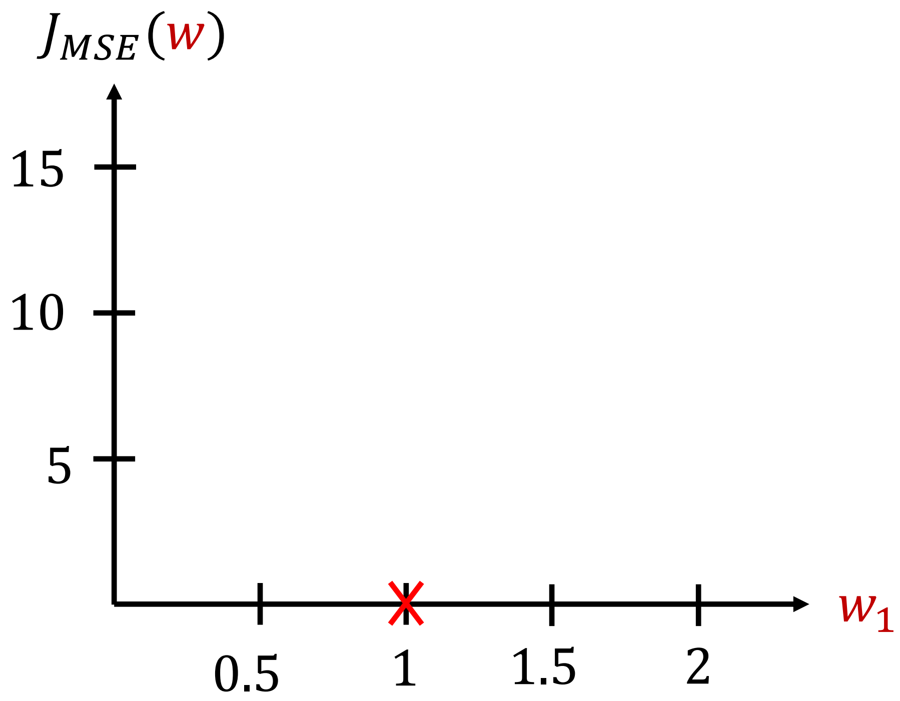
Linear Regression: Loss Landscape

Simplify: fix to 0!

Hypothesis:

$$h_w(x) = \boxed{0} + w_1 x$$





Loss Function:

$$J_{MSE}(w) = \frac{1}{2m}\sum_{i=1}^{m}\left(w_1 x^{(i)} - y^{(i)}\right)^2$$

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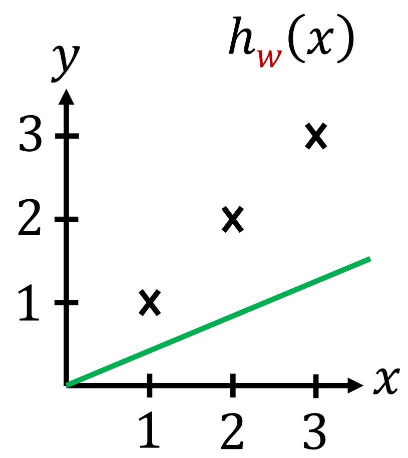
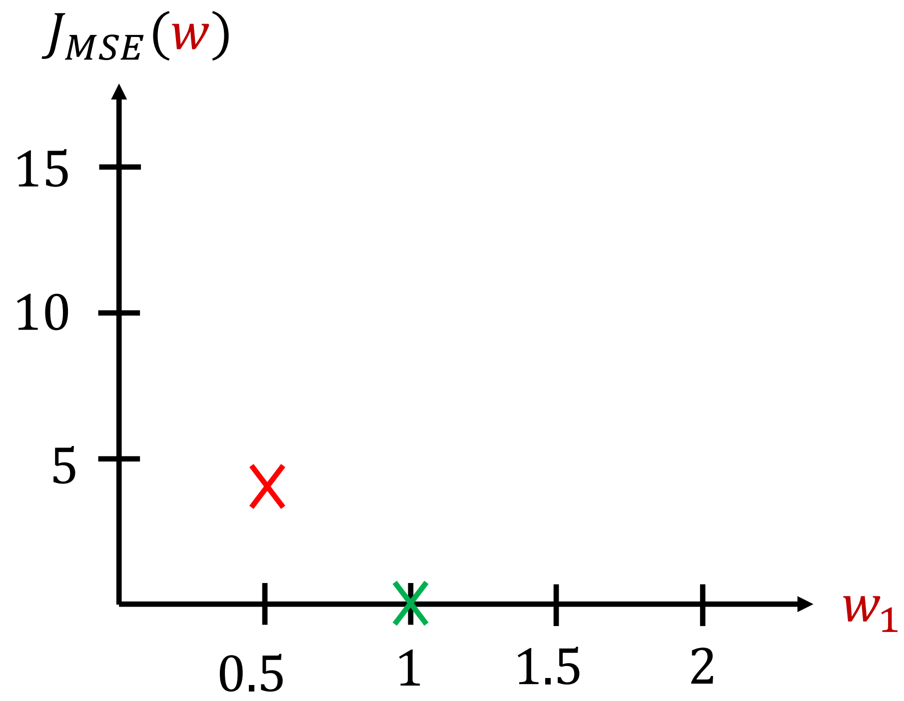




Loss Function:

$$J_{MSE}(w) = \frac{1}{2m}\sum_{i=1}^{m}\left(w_1 x^{(i)} - y^{(i)}\right)^2$$

$= (1\text{-}0.5)^2 + (2\text{-}1)^2 + (3\text{-}1.5)^2$

$= 0.5^2 + 1 + (1.5)^2$

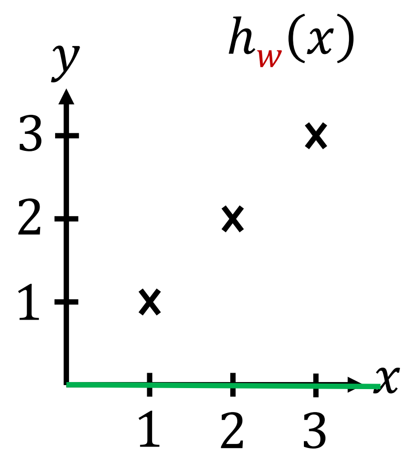
$= 3.5$

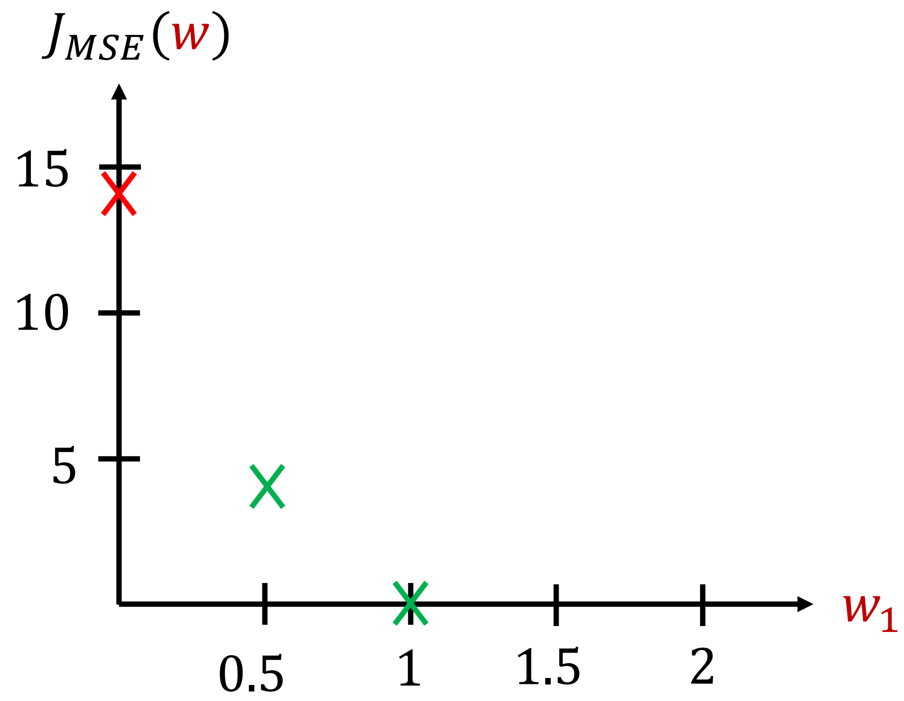
Linear Regression: Loss Landscape

Simplify: fix to 0!

Hypothesis:

$$h_w(x) = \boxed{0} + w_1 x$$





Loss Function:

$$J_{MSE}(w) = \frac{1}{2m}\sum_{i=1}^{m}\left(w_1 x^{(i)} - y^{(i)}\right)^2$$

$= 1^2 + 2^2 + 3^2$

$= 14$

Linear Regression: Loss Landscape

Simplify: fix to 0!

Hypothesis:

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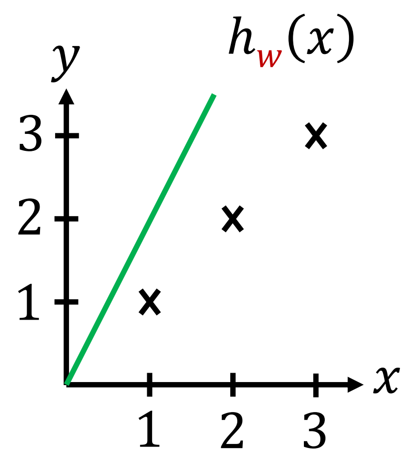

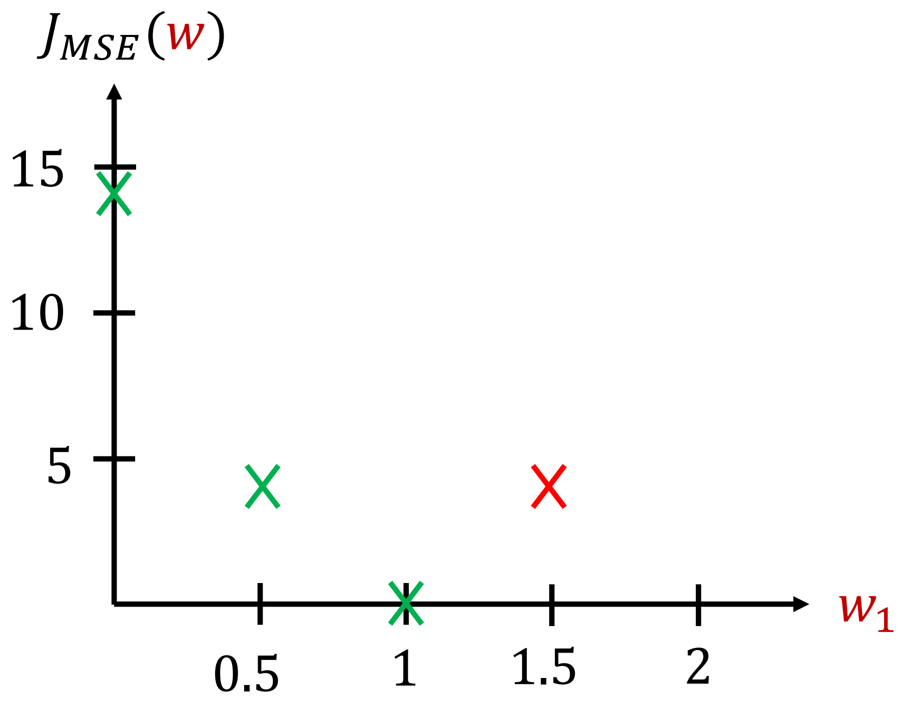

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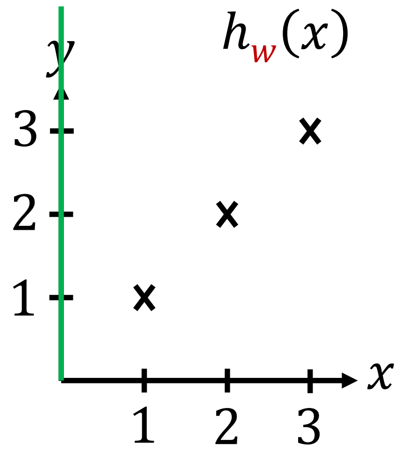

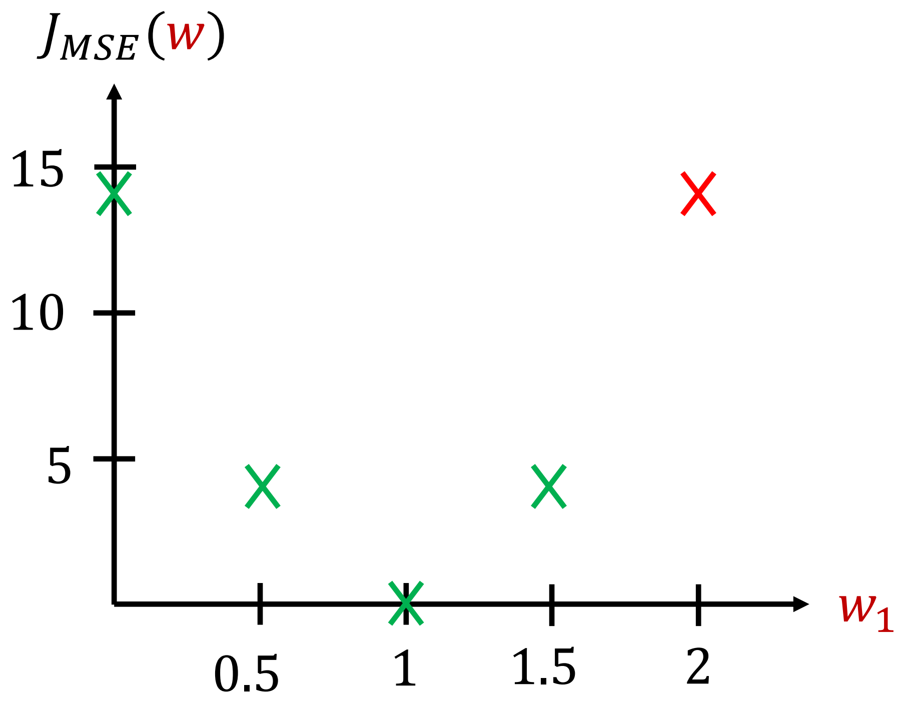

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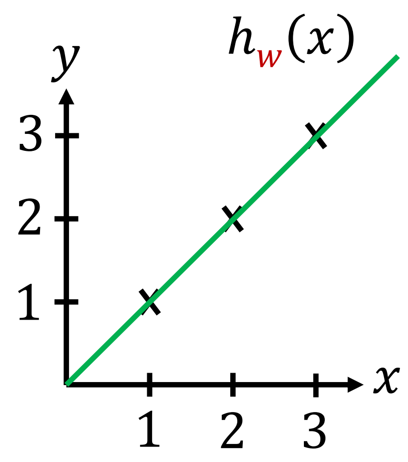

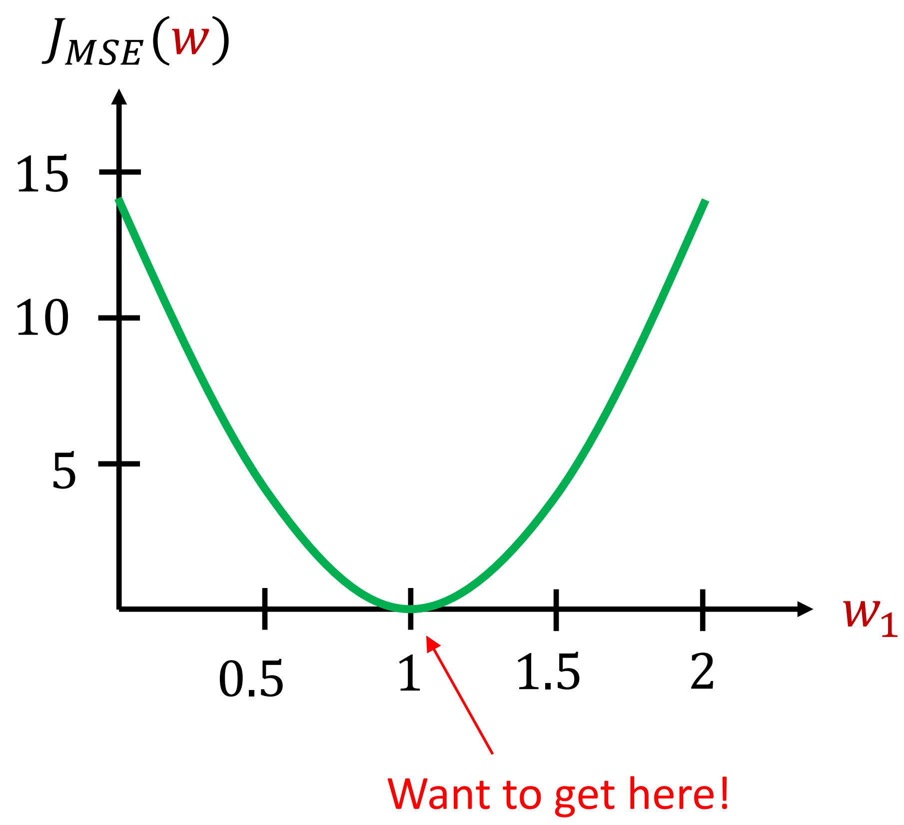

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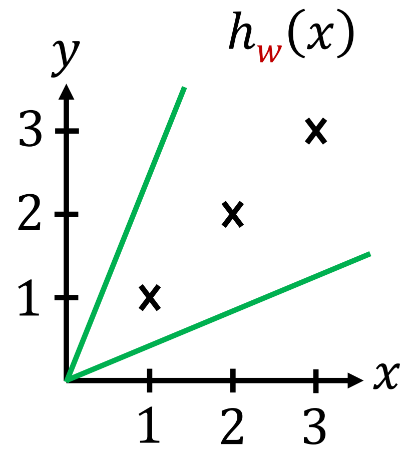

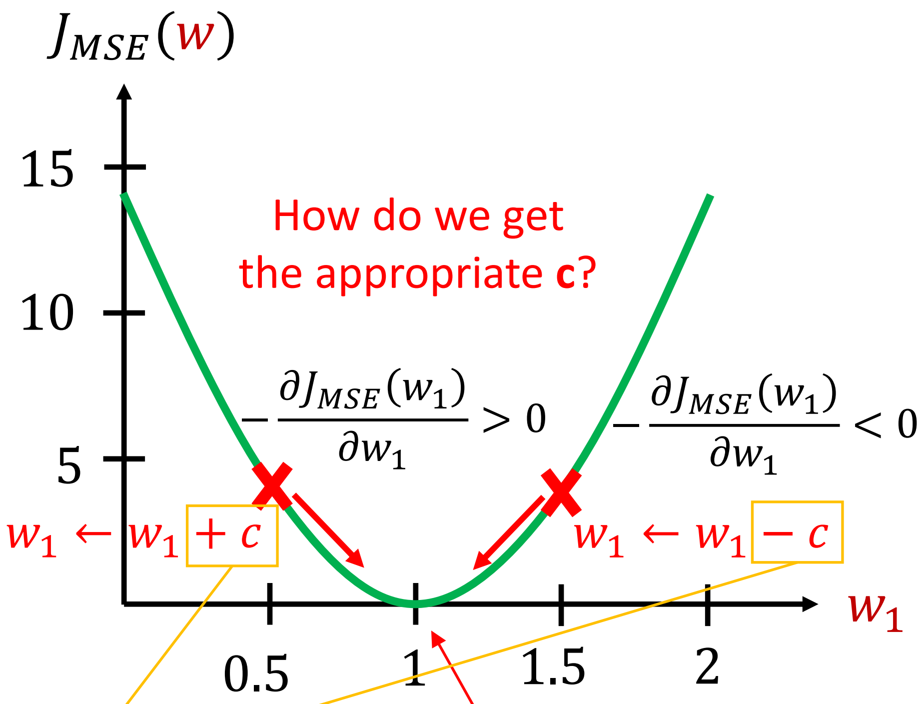

Want to get here!

Loss Function:

$$J_{MSE}(w) = \frac{1}{2m} \sum_{i=1}^{m} \left(w_1 x^{(i)} - y^{(i)} \right)^2$$

$$\frac{\partial J_{MSE}(w)}{\partial w} = \frac{1}{m} \sum_{i=1}^{m} (w_1 x^{(i)} - y^{(i)}) x^{(i)}$$

(0.5*1 - 1)*1 = -0.5

(1.5*1 - 1)*1 = +0.5

$$w_1 \leftarrow w_1 \boxed{- \gamma \frac{\partial J_{MSE}(w_1)}{\partial w_1}}$$

+ve constant

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Gradient Descent

Remember Hill-climbing?

- Start at some w
- Pick a nearby point that reduces $J(w)$

$$w_j \leftarrow w_j - \gamma \frac{\partial J(w_0, w_1, \dots)}{\partial w_j}$$

- Repeat until minimum is reached

Learning Rate

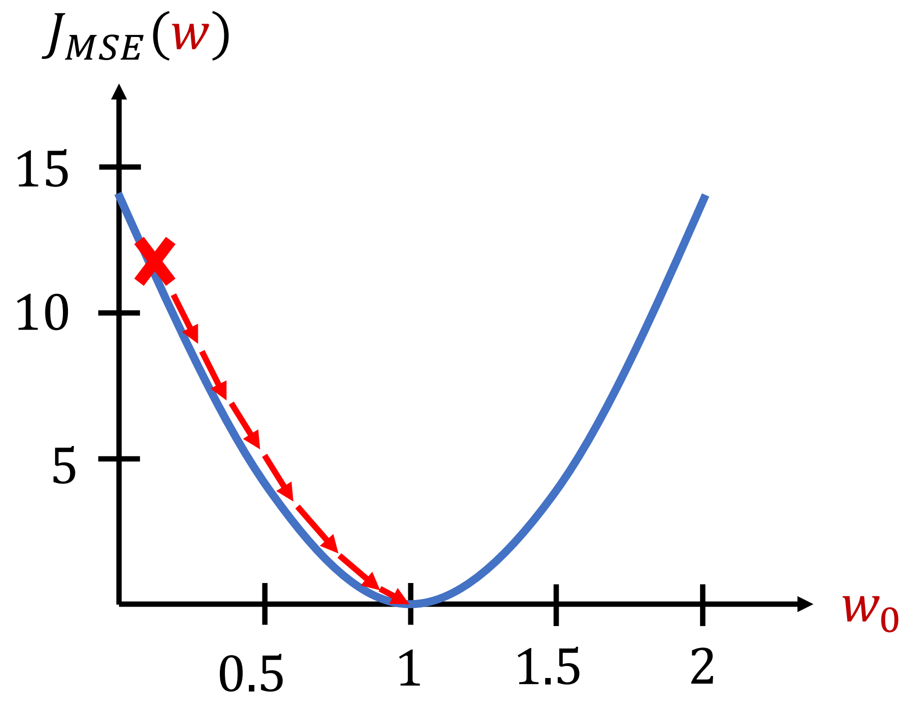
Gradient Descent: 1 Parameter

- Start at some w_0
- Pick a nearby point that reduces $J(w_0)$

$$w_0 \leftarrow w_0 - \gamma \boxed{\frac{\partial J(w_0)}{\partial w_0}}$$

- Repeat until minimum is reached

Learning Rate



As it gets closer to a minimum,
- The **gradient** becomes smaller
- The **steps** becomes smaller

Can we use mean absolute error (MAE) for our J?

MAE is <u>not</u> **fully differentiable** (its derivative is undefined at 0)

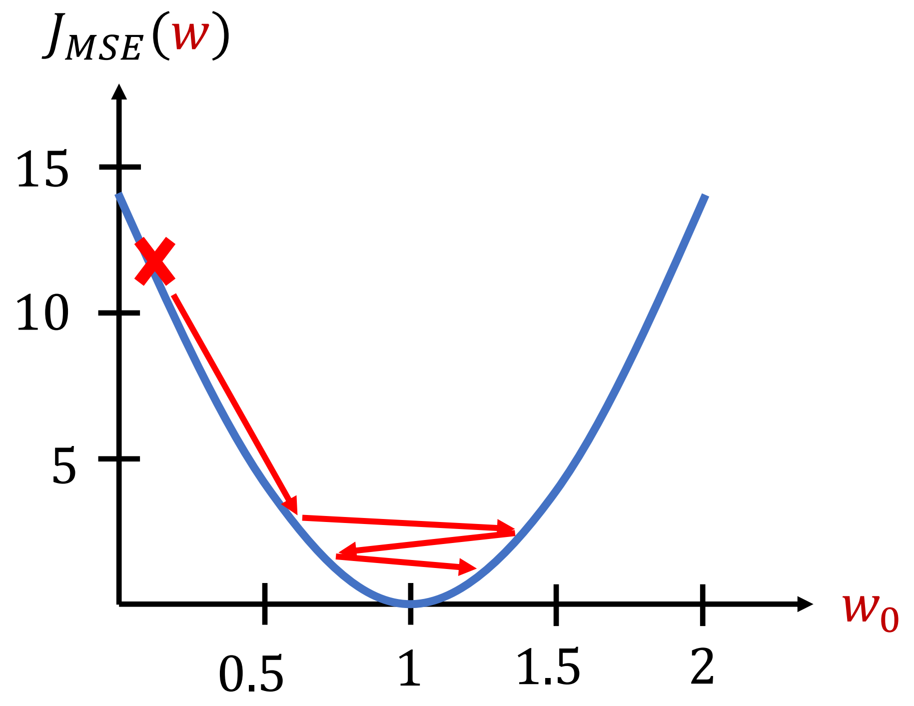
Gradient Descent: 1 Parameter

- Start at some w_0
- Pick a nearby point that reduces $J(w_0)$

$$w_0 \leftarrow w_0 - \gamma \frac{\partial J(w_0)}{\partial w_0}$$

- Repeat until minimum is reached

Learning Rate



γ too large

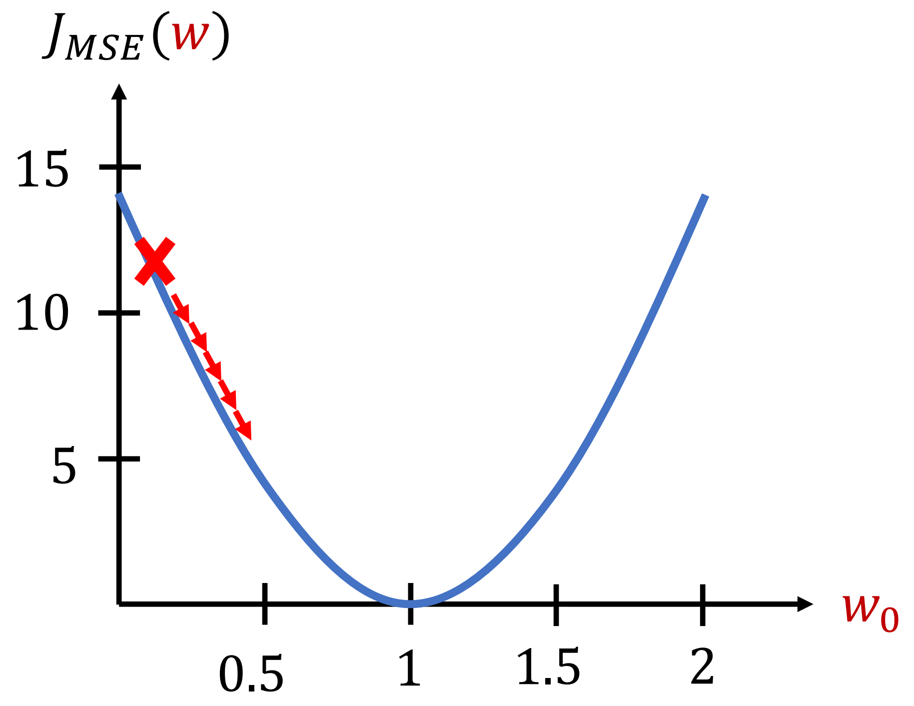
Gradient Descent: 1 Parameter

- Start at some w_0
- Pick a nearby point that reduces $J(w_0)$

$$w_0 \leftarrow w_0 - \gamma \frac{\partial J(w_0)}{\partial w_0}$$

Learning Rate

- Repeat until minimum is reached



γ too small

Gradient Descent: 2 Parameters

- Start at some $w = (w_0, w_1)$
- Pick a nearby point that reduces $J(w)$

$$w_j \leftarrow w_j - \gamma \frac{\partial J(w_0, w_1)}{\partial w_j}$$

- Repeat until minimum is reached

Learning Rate

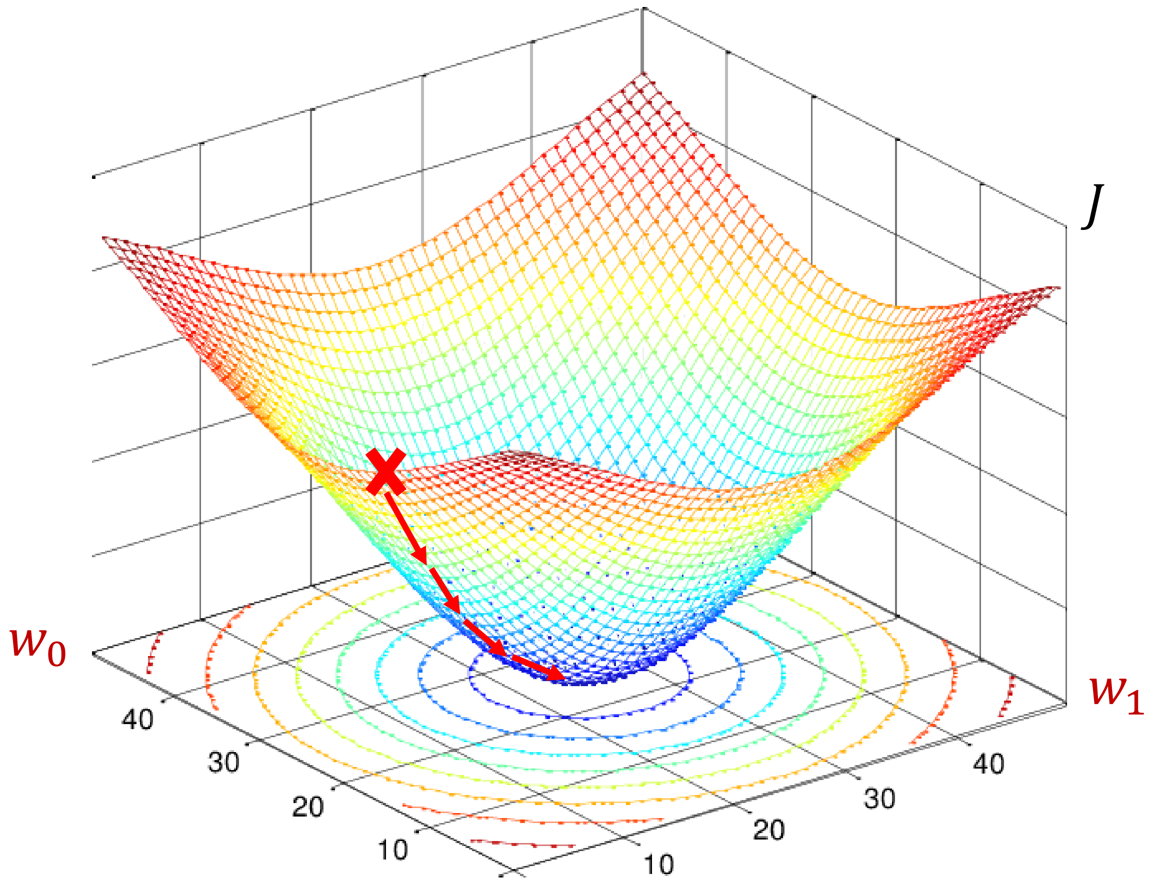


Image Credit: https://www.researchgate.net/figure/The-2D-Caussian-function-of-Example-2-Example-1-Consider-the-following-strongly-convex_fig2_230787652

Gradient Descent

- Start at some w
- Pick a nearby point that reduces $J(w)$

$$w_j \leftarrow w_j - \gamma \frac{\partial J(w_0, w_1, \dots)}{\partial w_j}$$

Learning Rate

- Repeat until minimum is reached

Common Mistakes

w_0 changed!

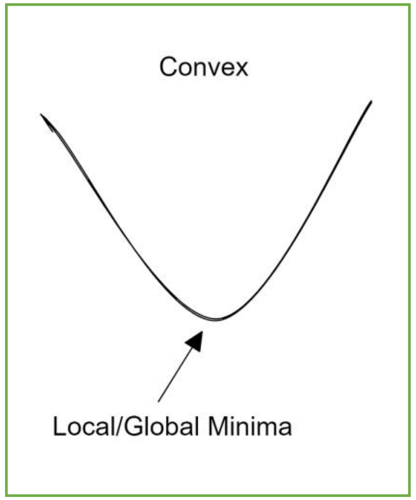
$$w_0 = w_0 + \gamma \frac{\partial J(w_0, w_1)}{\partial w_0}$$
$$w_1 = w_1 + \gamma \frac{\partial J(w_0, w_1)}{\partial w_1}$$

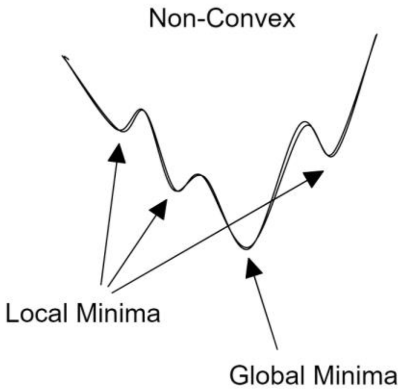
$$a = \frac{\partial J(w_0, w_1)}{\partial w_0}$$
$$b = \frac{\partial J(w_0, w_1)}{\partial w_1}$$
$$w_0 = w_0 + \gamma a$$
$$w_1 = w_1 + \gamma b$$

Linear Regression with Gradient Descent

Hypothesis:

$h_w(x) = w_0 + w_1 x$





Loss Function:

$$J_{MSE}(w_0, w_1) = \frac{1}{2m}\sum_{i=1}^{m}(w_0 + w_1 x^{(i)} - y^{(i)})^2$$

$$\frac{\partial J_{MSE}(w_0, w_1)}{\partial w_j} = \frac{\partial}{\partial w_j}\frac{1}{2m}\sum_{i=1}^{m}(w_0 + w_1 x^{(i)} - y^{(i)})^2$$

$$\frac{\partial J_{MSE}(w_0, w_1)}{\partial w_0} = \frac{1}{m}\sum_{i=1}^{m}(w_0 + w_1 x^{(i)} - y^{(i)})$$

$$\frac{\partial J_{MSE}(w_0, w_1)}{\partial w_1} = \frac{1}{m}\sum_{i=1}^{m}(w_0 + w_1 x^{(i)} - y^{(i)}).x^{(i)}$$

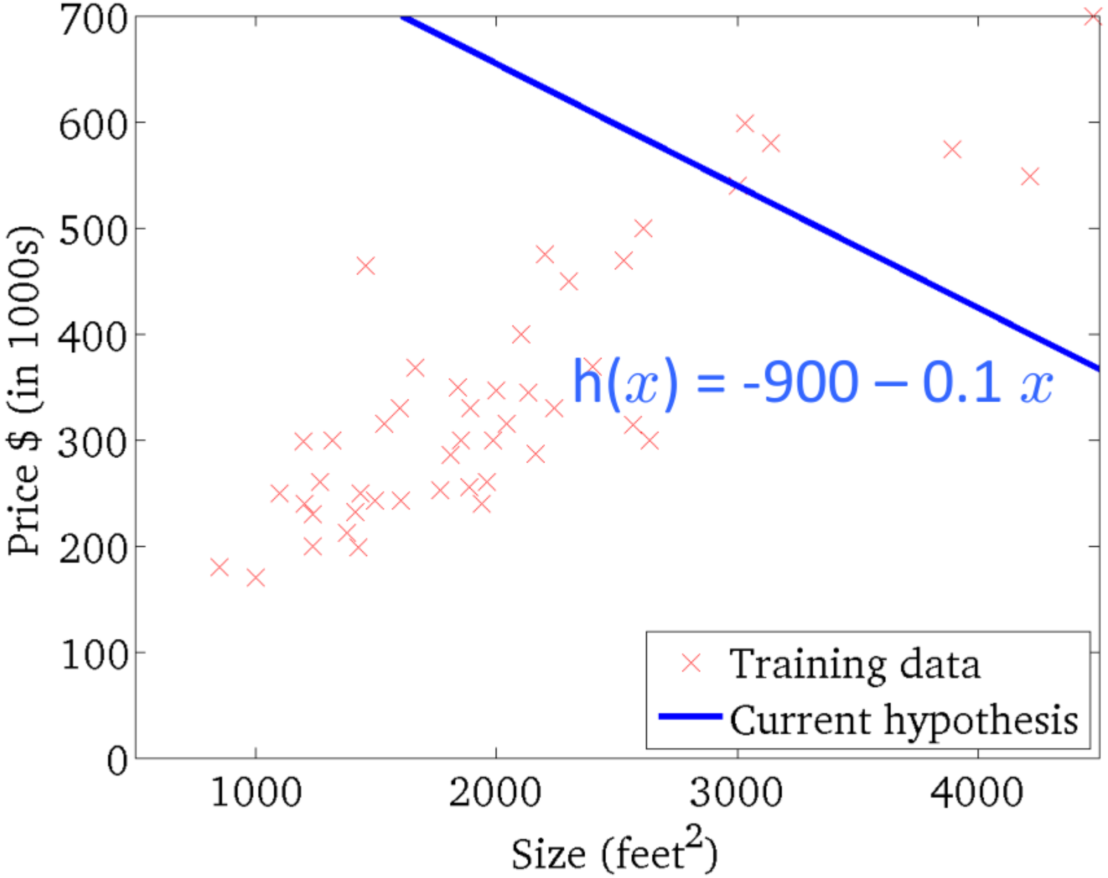
Theorem: MSE loss function is convex for linear regression.

- One minimum, global minimum

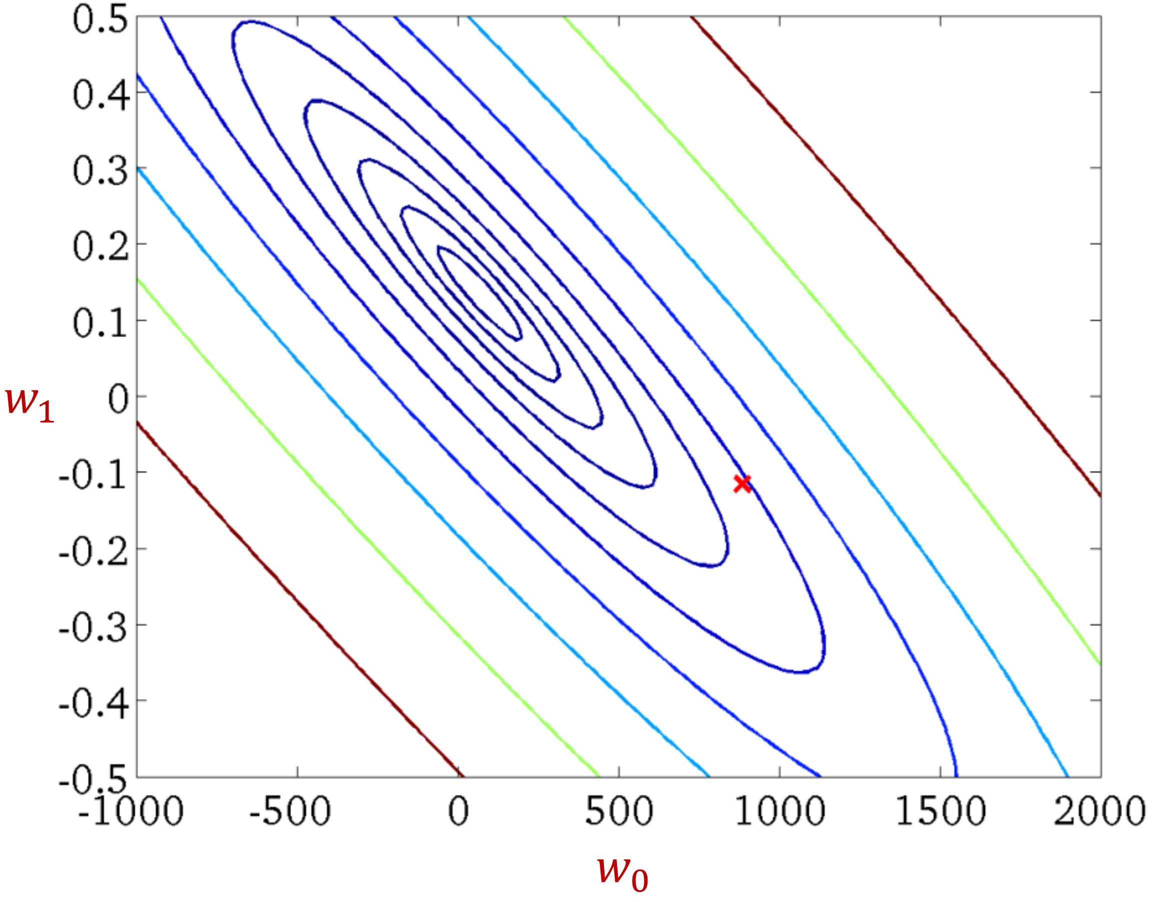
Image Credit: https://python.plainenglish.io/logistic-regression-in-machine-learning-from-scratch-872b1fedd05b

Linear Regression with Gradient Descent

$h_w(x)$



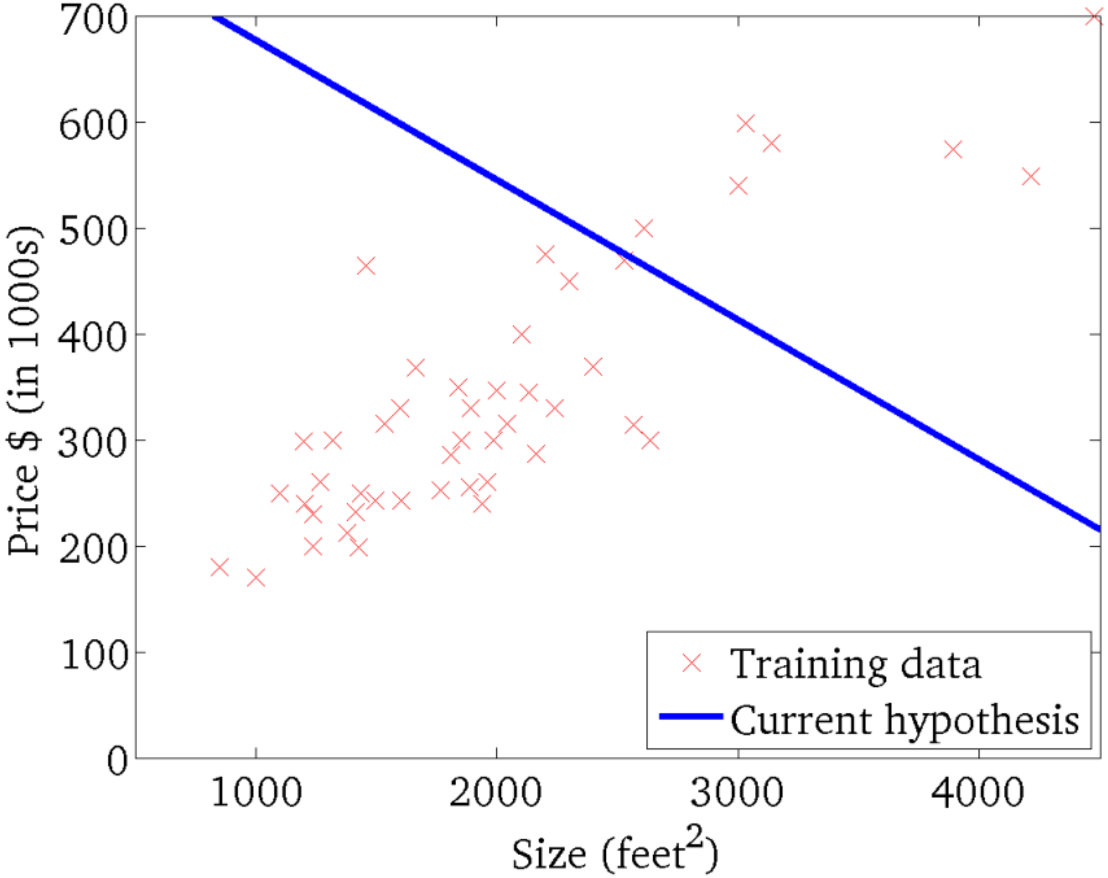
$J_{MSE}(w_0, w_1)$



Credit: Andrew Ng

Linear Regression with Gradient Descent

$h_w(x)$



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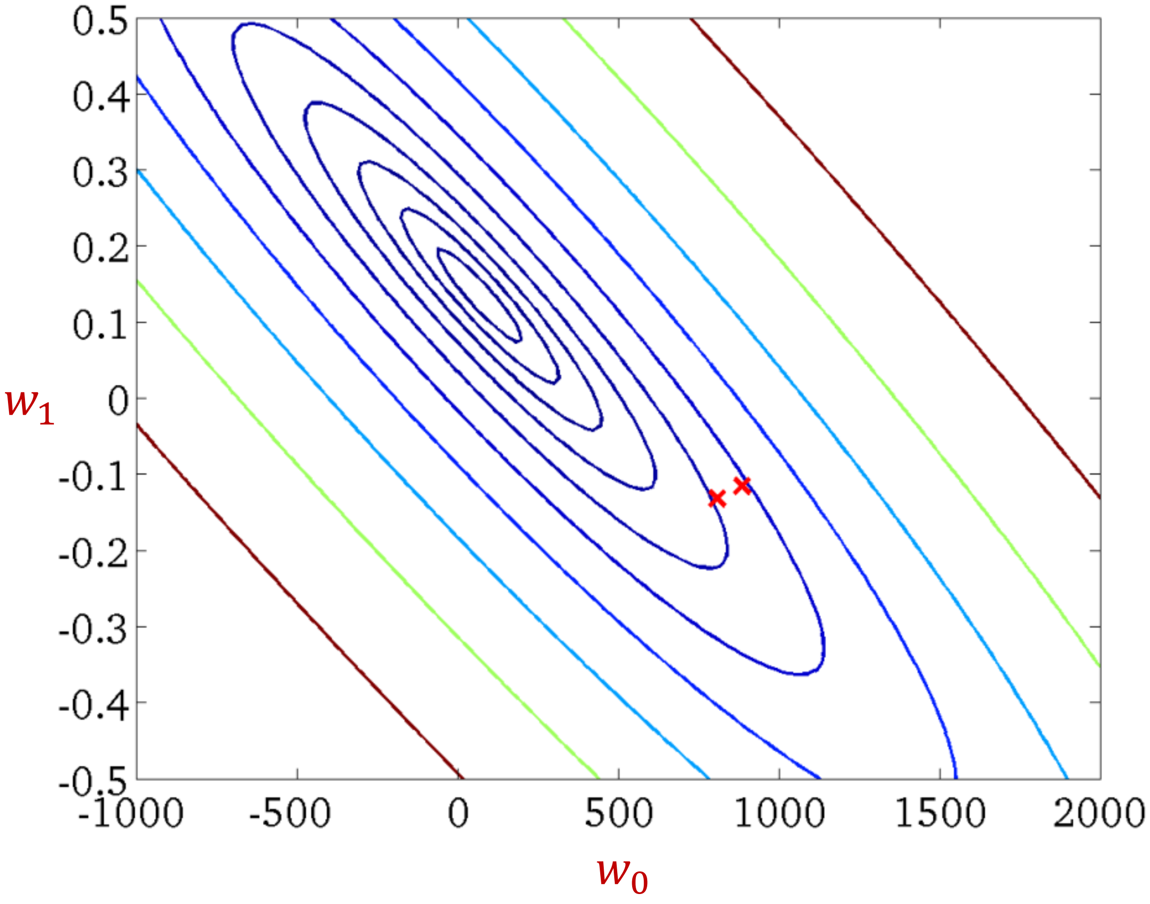

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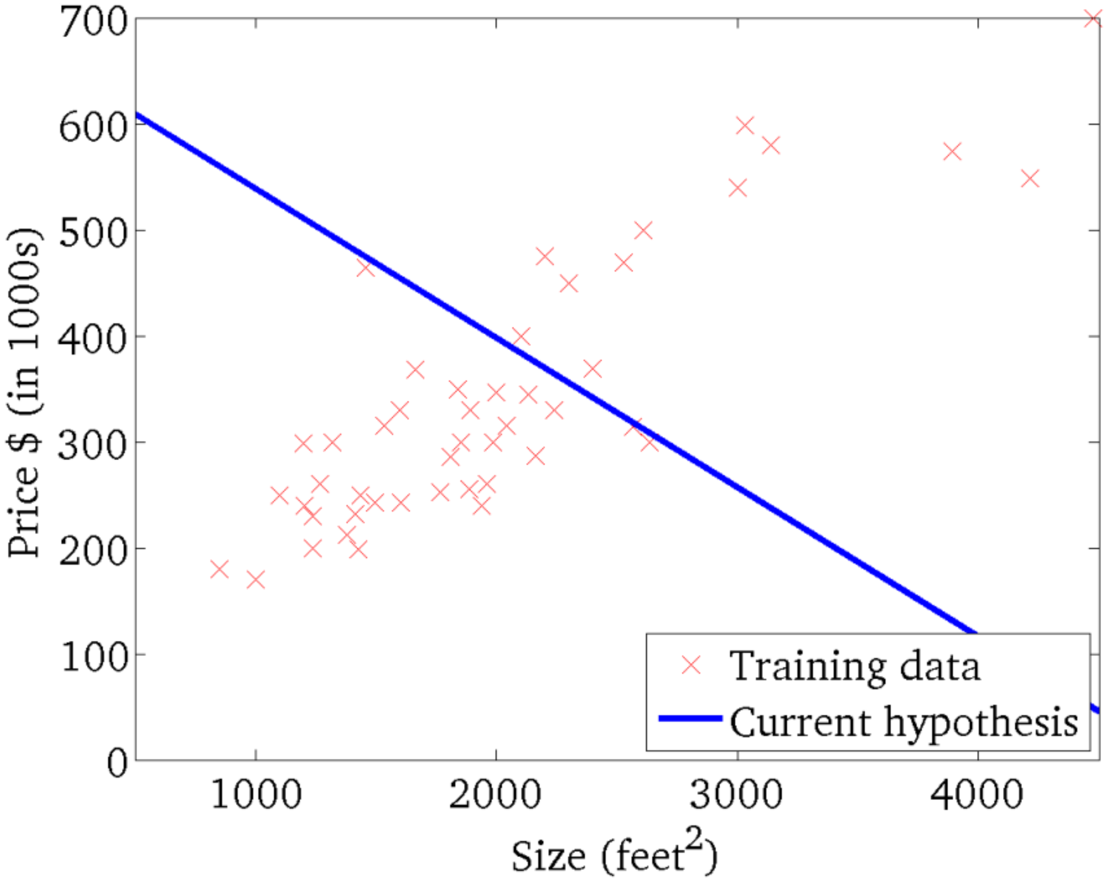
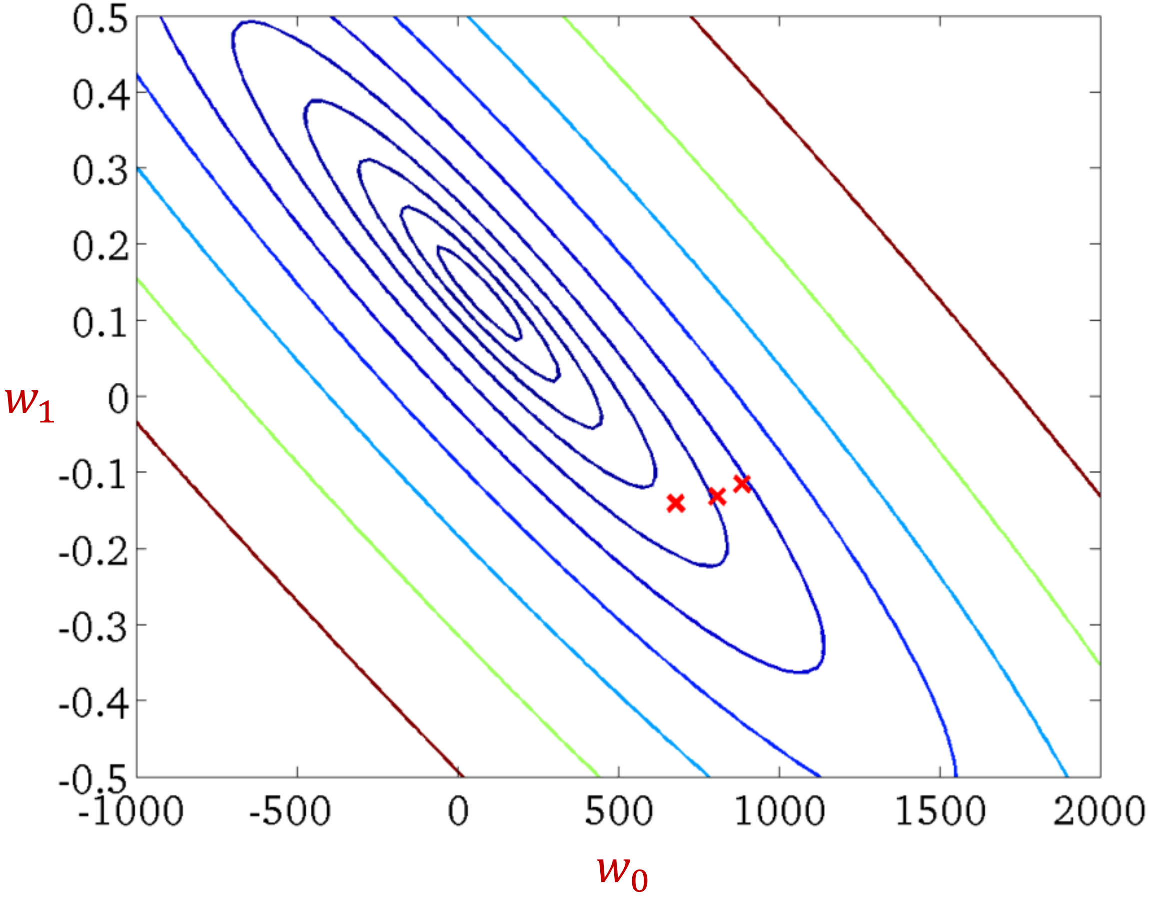
Linear Regression with Gradient Descent

$h_w(x)$



$J_{MSE}(w_0, w_1)$



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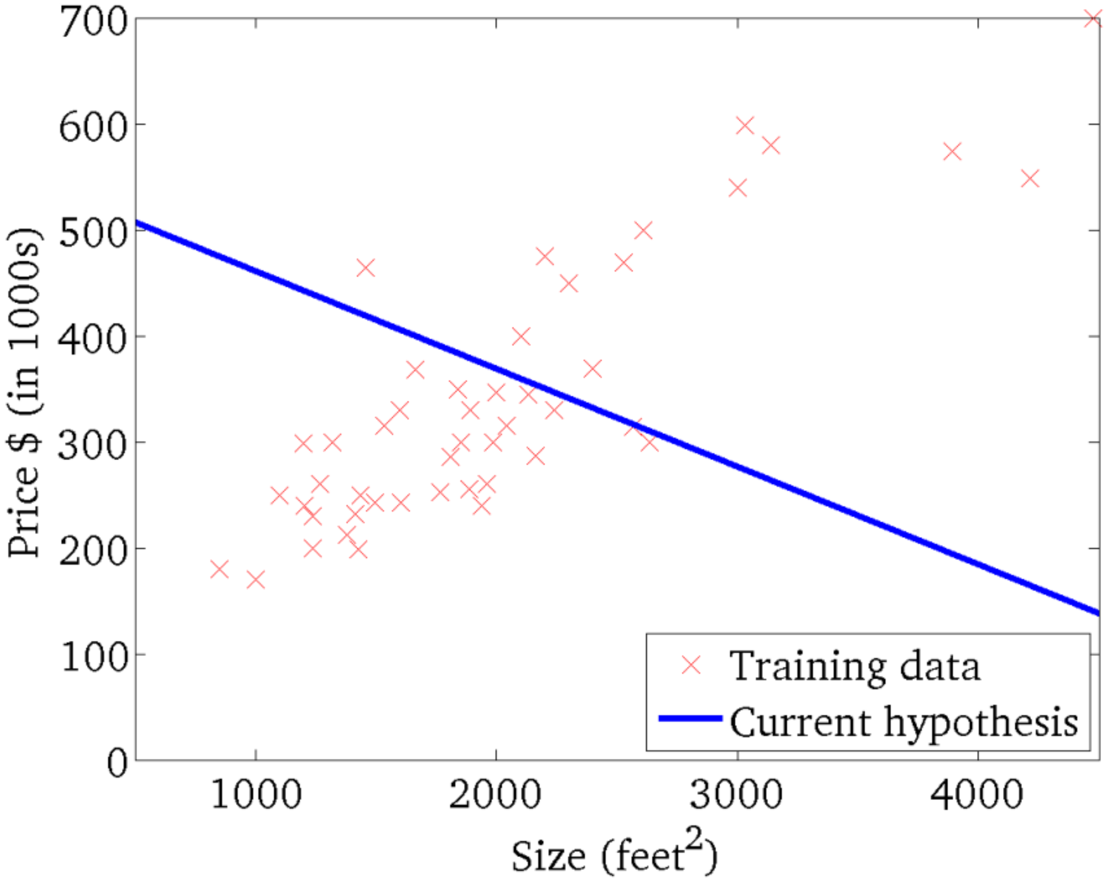
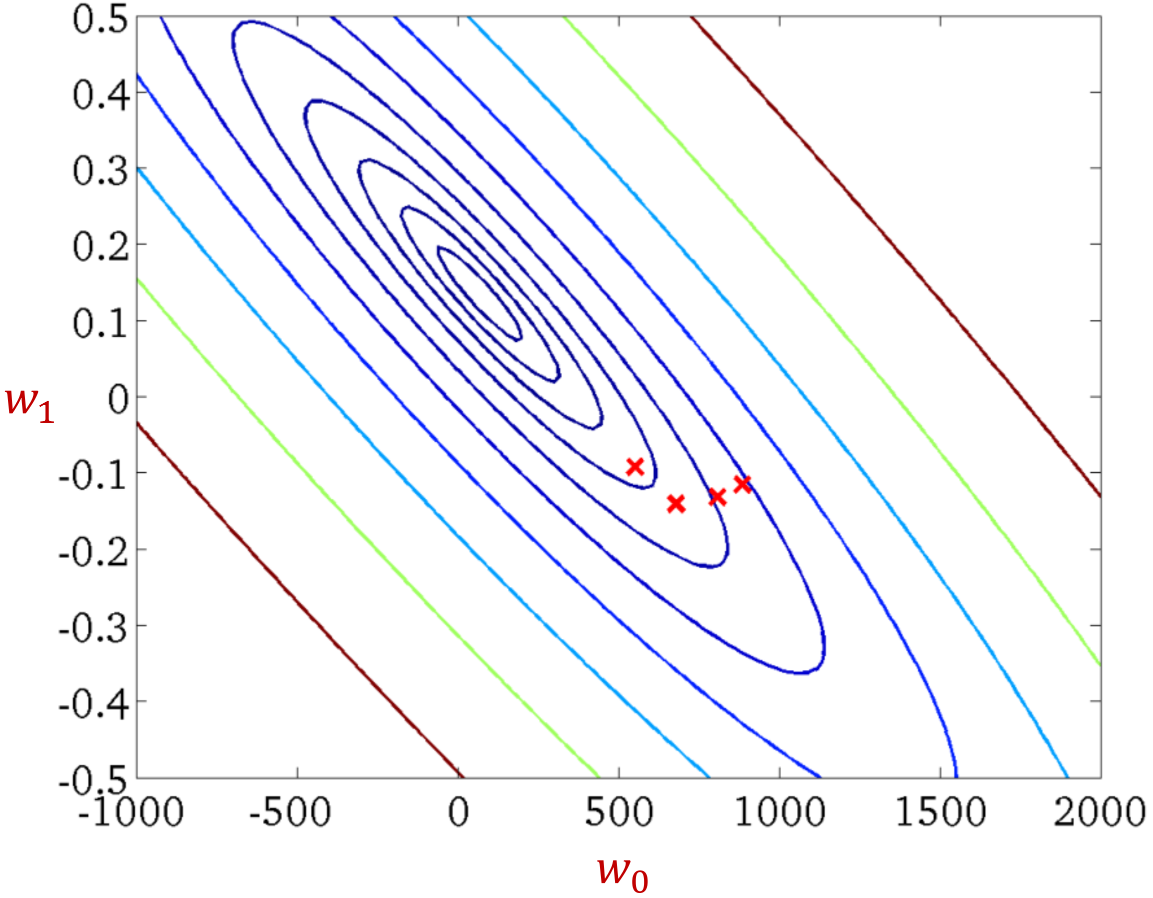
Linear Regression with Gradient Descent

$h_w(x)$



$J_{MSE}(w_0, w_1)$



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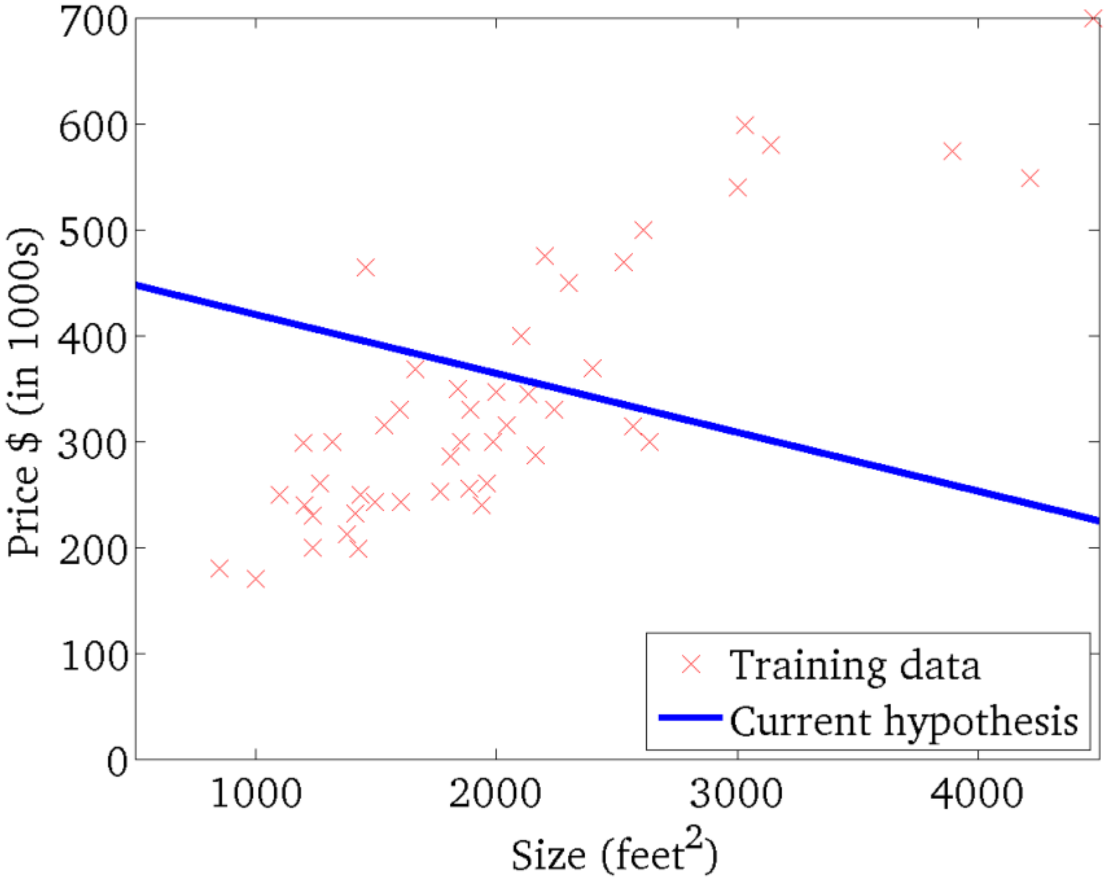
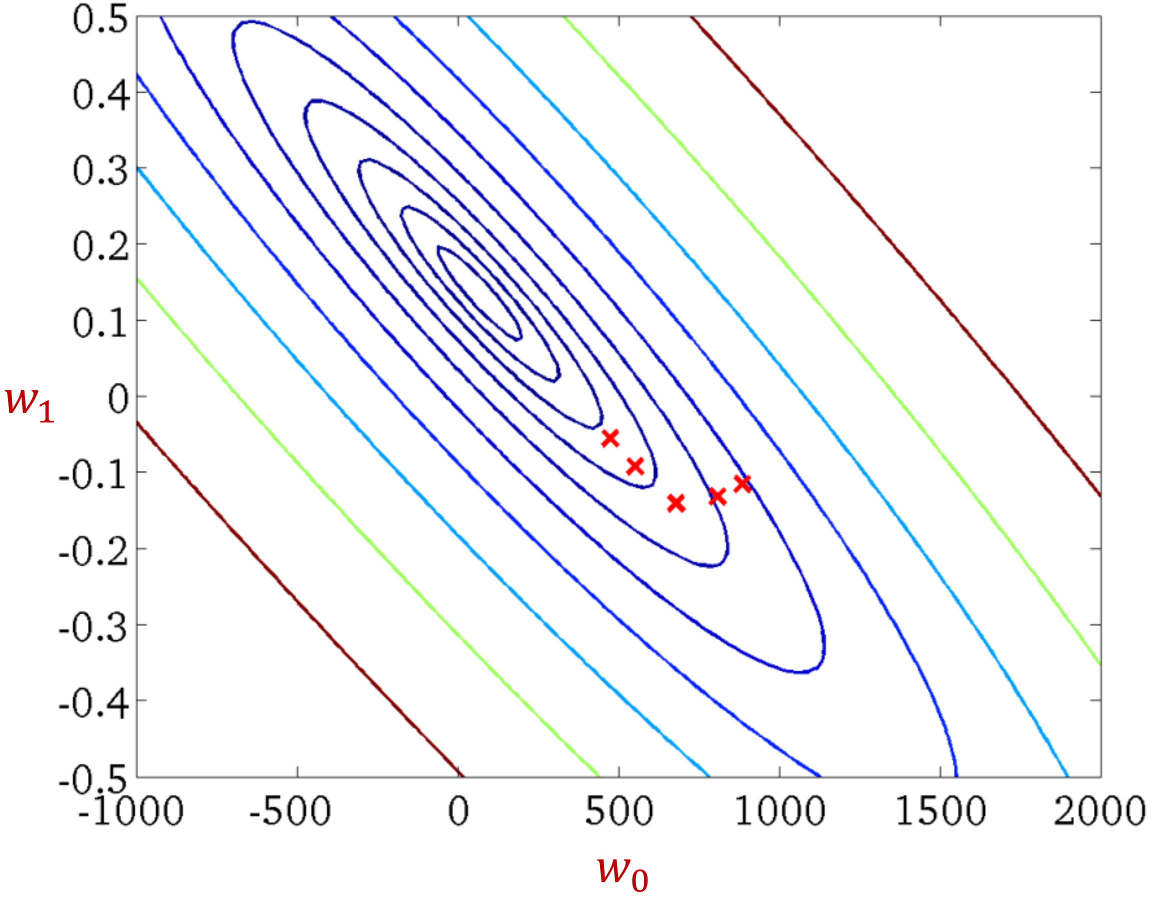
Linear Regression with Gradient Descent

$h_w(x)$



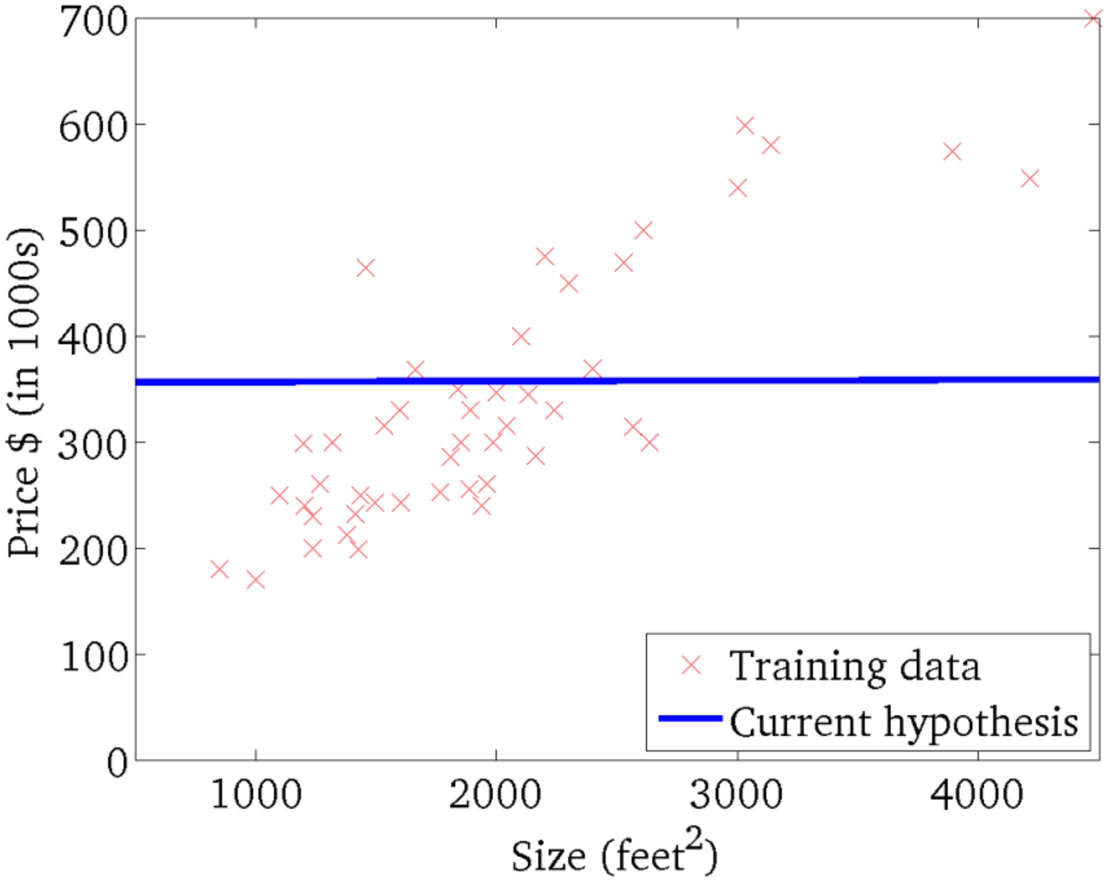
$J_{MSE}(w_0, w_1)$



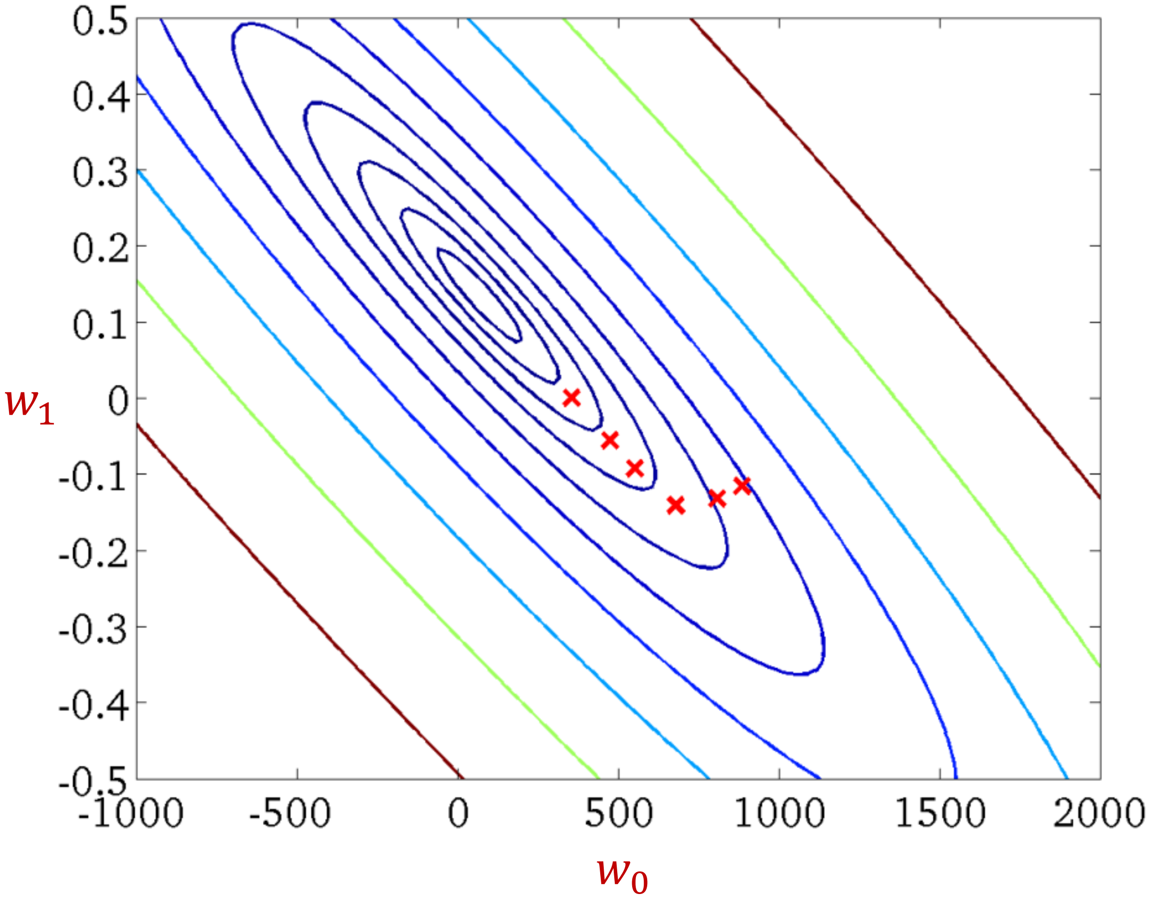
Credit: Andrew Ng

Linear Regression with Gradient Descent

$h_w(x)$

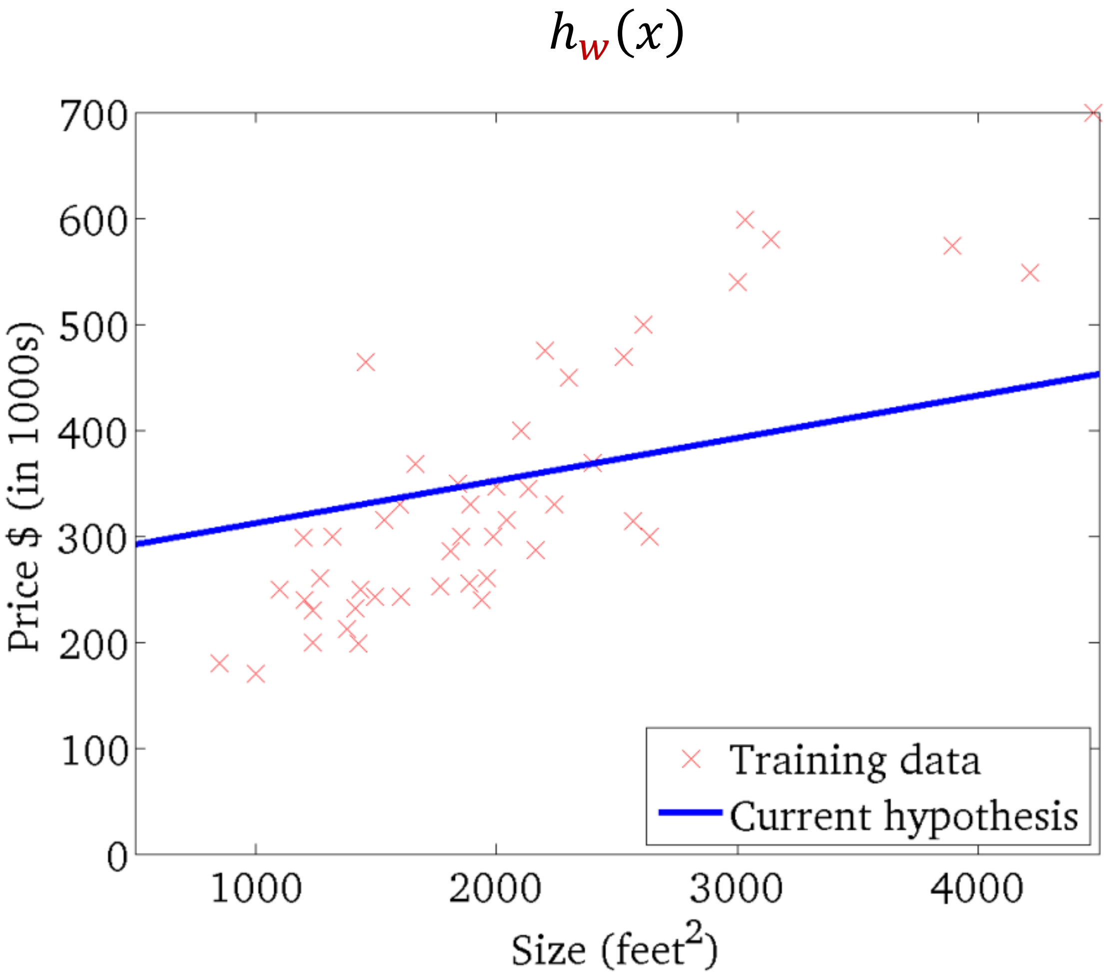


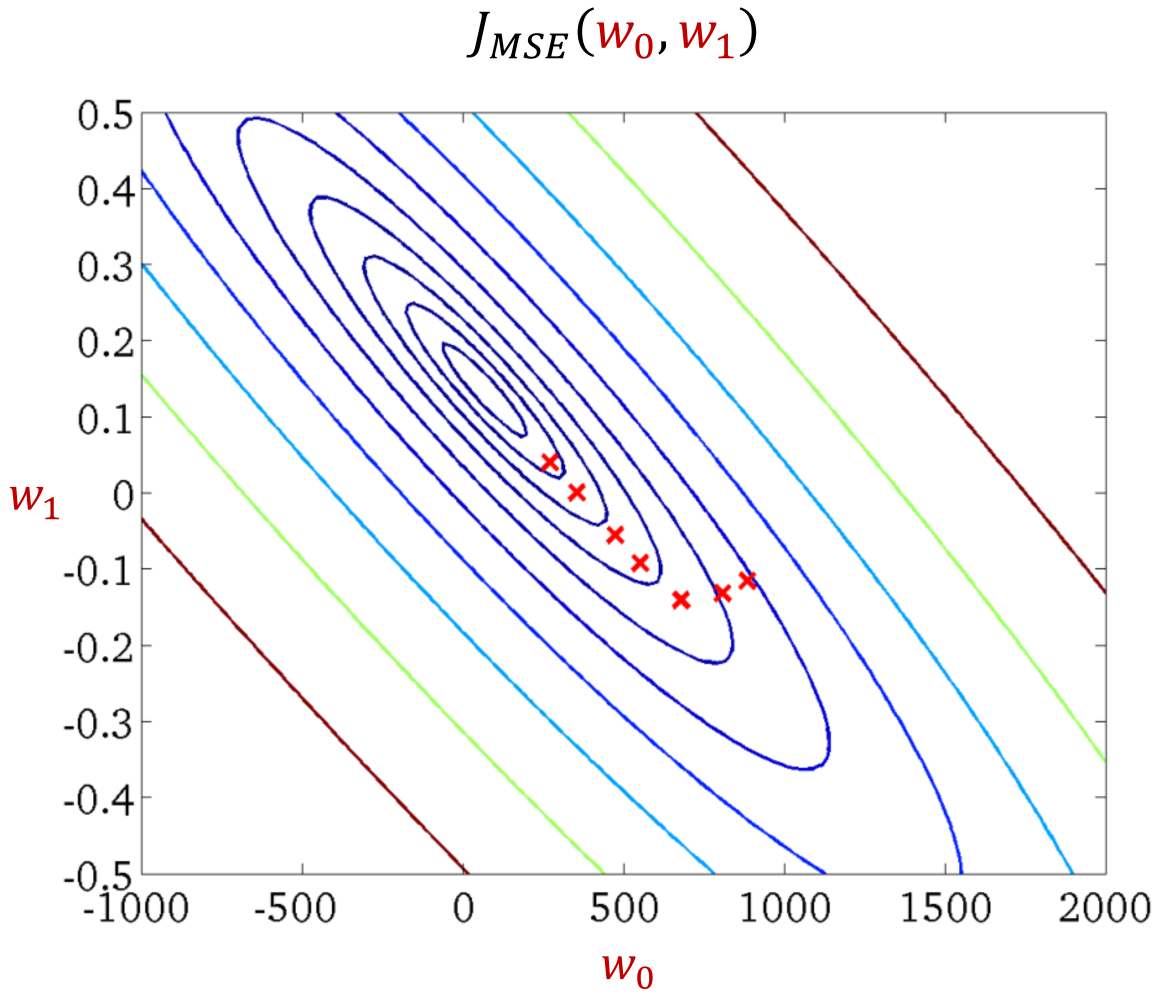
$J_{MSE}(w_0, w_1)$



Credit: Andrew Ng

Linear Regression with Gradient Descent

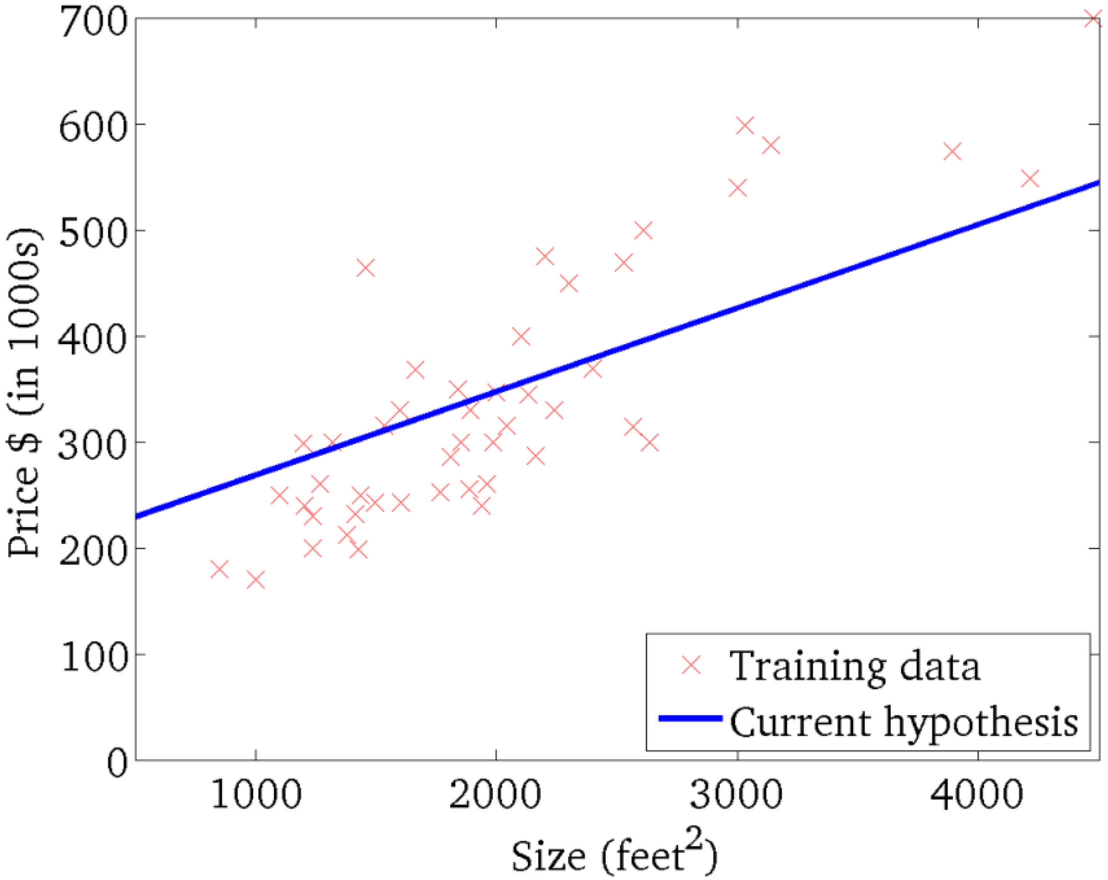




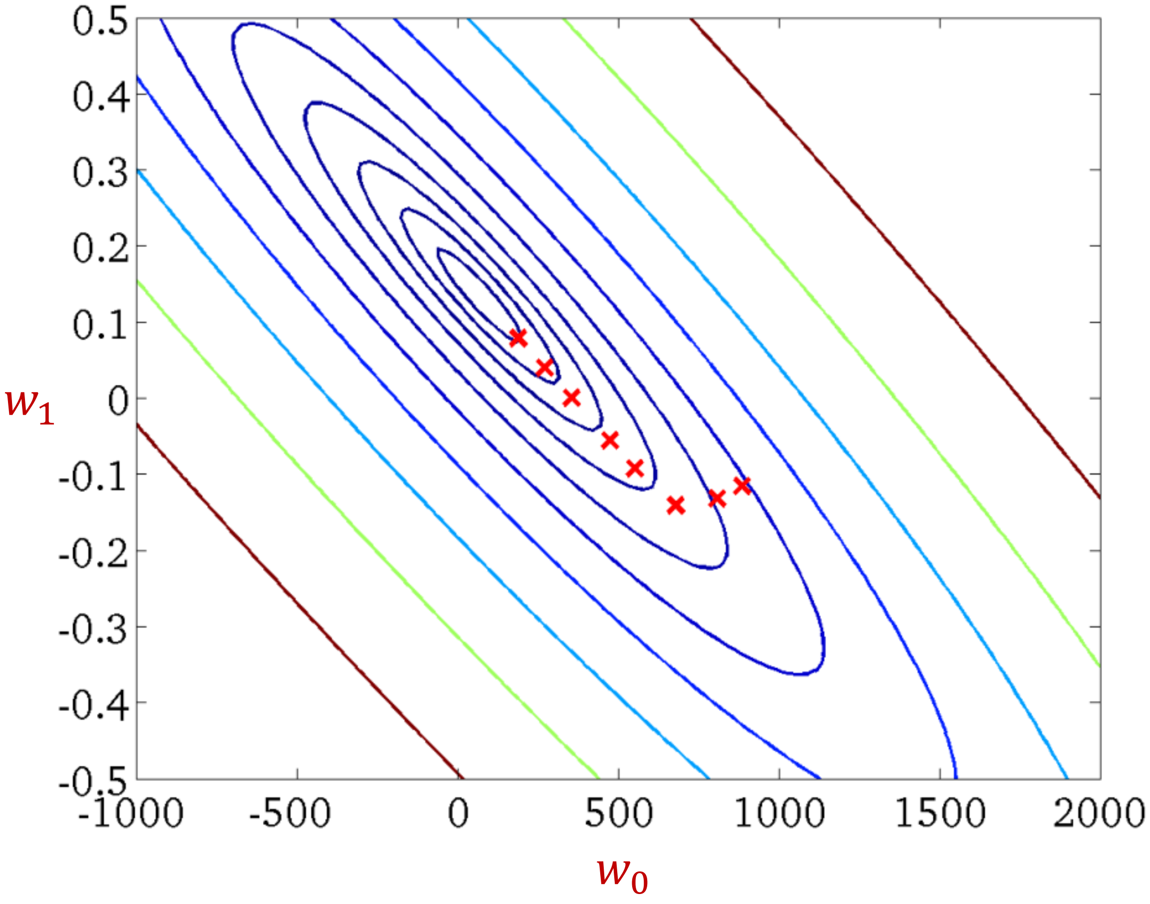
Credit: Andrew Ng

Linear Regression with Gradient Descent

$h_w(x)$



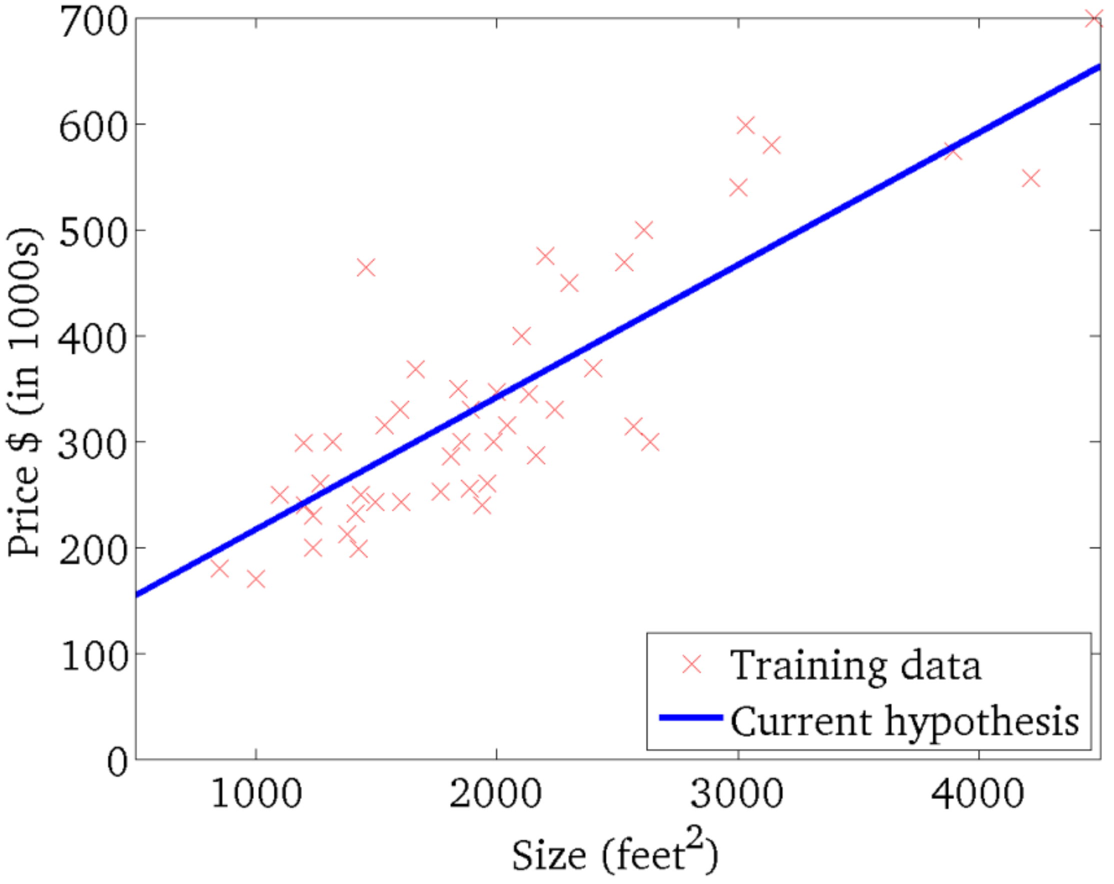
$J_{MSE}(w_0, w_1)$



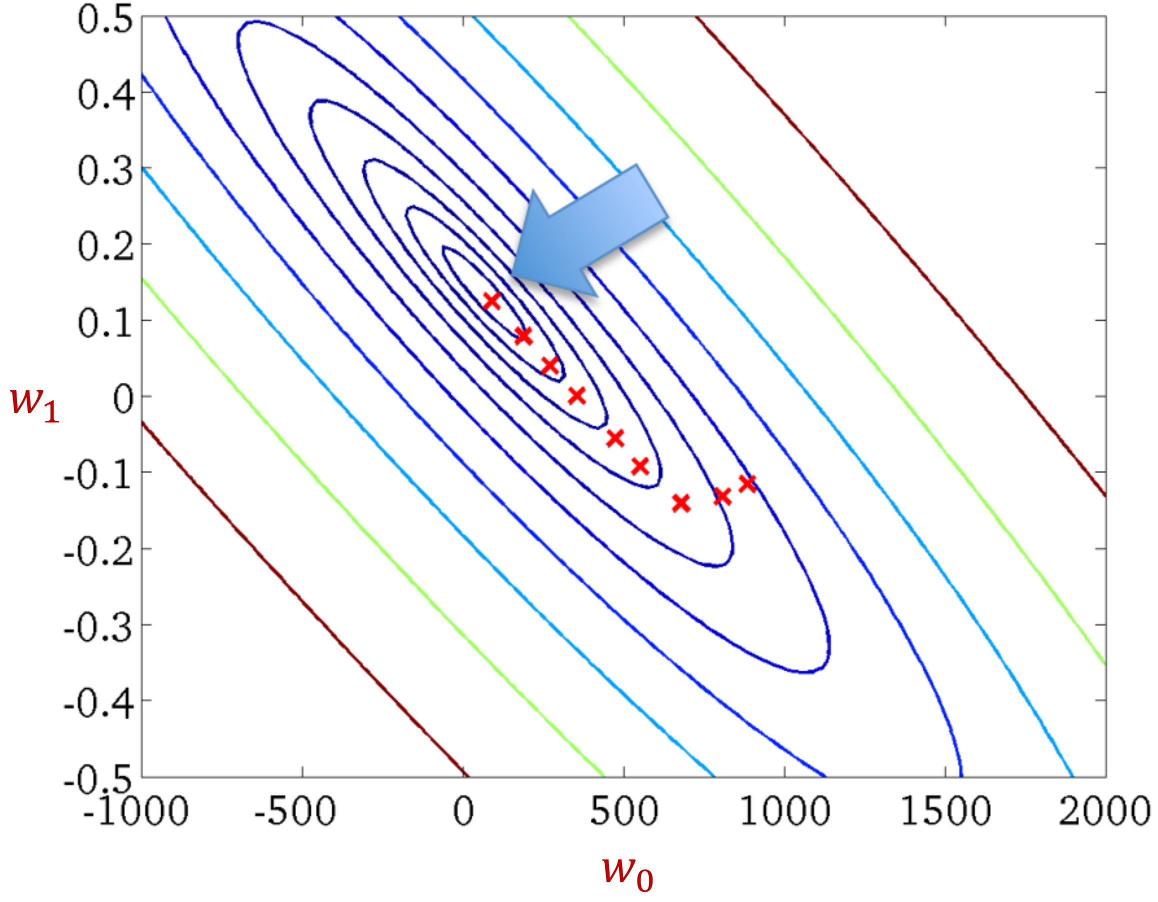
Credit: Andrew Ng

Linear Regression with Gradient Descent

$h_w(x)$

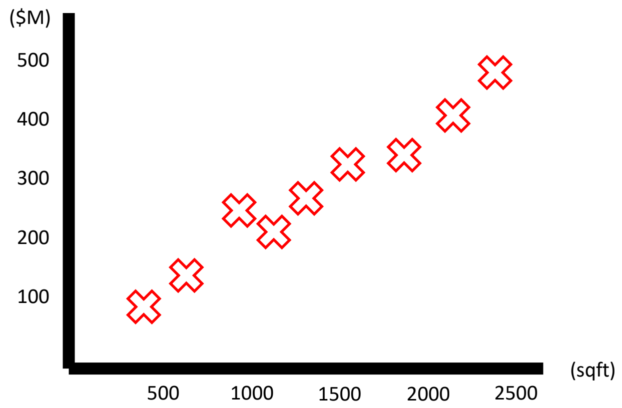


$J_{MSE}(w_0, w_1)$



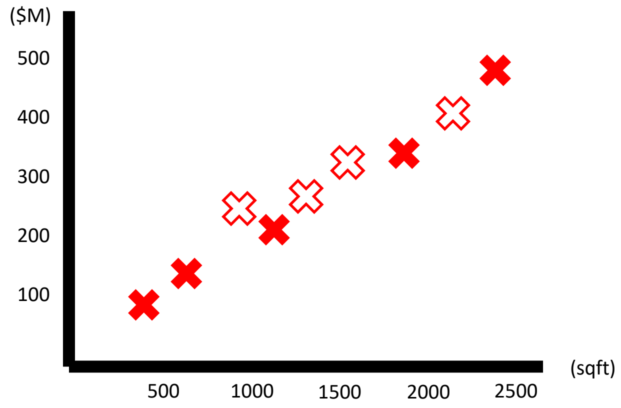
Credit: Andrew Ng

Variants of Gradient Descent



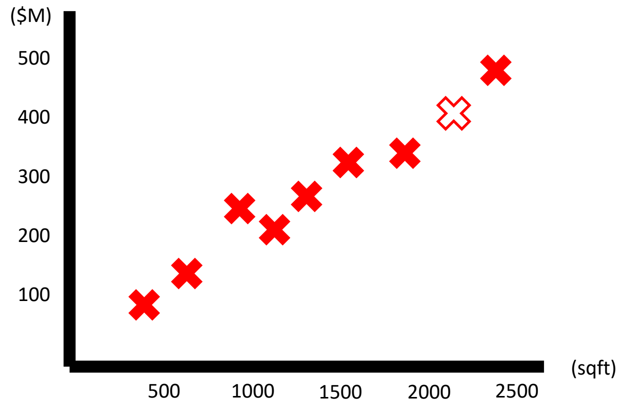
(Batch) Gradient Descent

- Consider all training examples



Mini-batch Gradient Descent

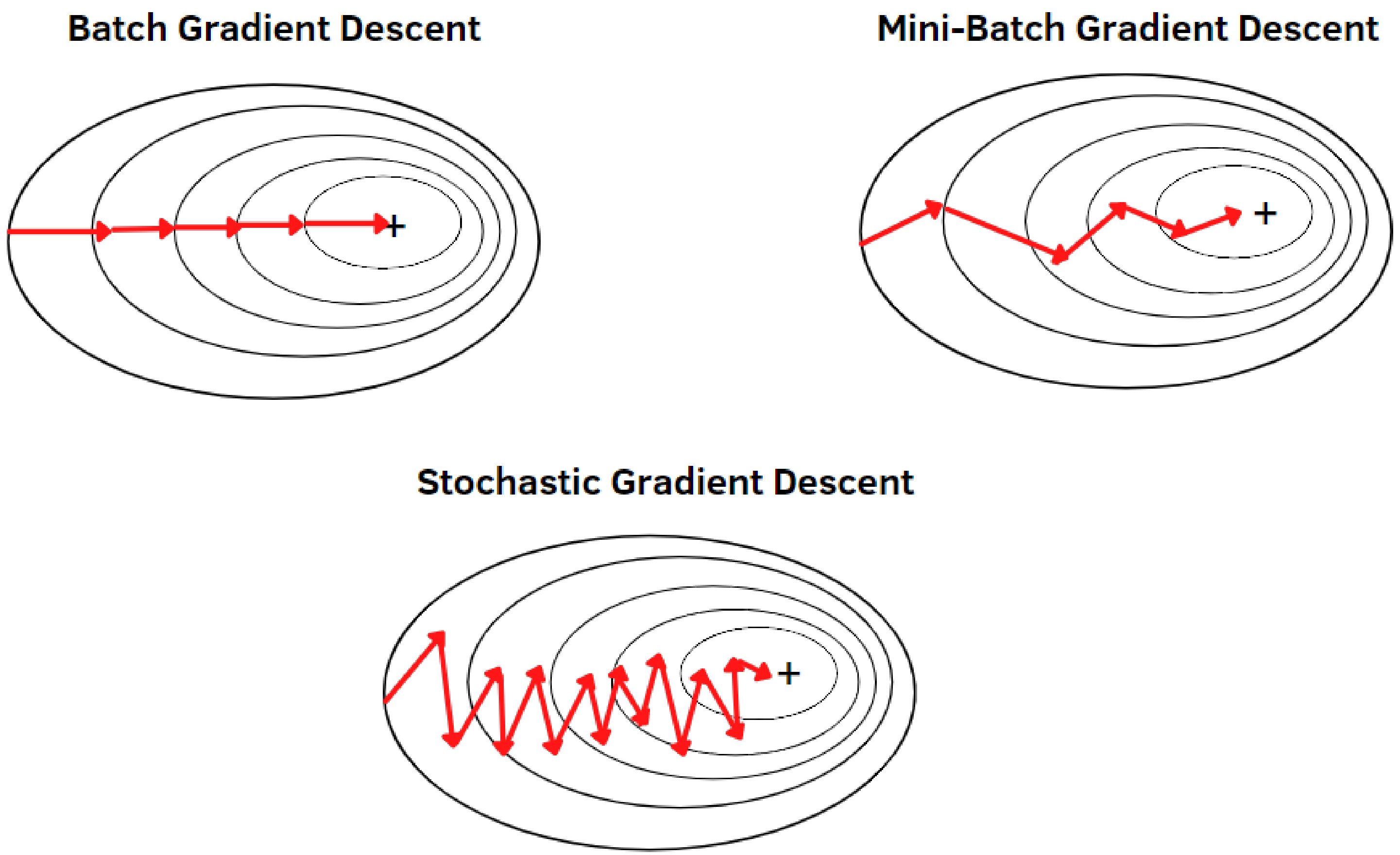
- Consider a subset of training examples at a time
- Cheaper (Faster) / iteration
- Randomness, may escape local minima



Stochastic Gradient Descent (SGD)

- Select one random data point at a time
- Cheapest (Fastest) / iteration
- More randomness, may escape local minima

Variants of Gradient Descent



Credit: analyticsvidhya.com

Outline

- Linear Regression
- Gradient Descent
  - Gradient Descent Algorithm
  - Linear Regression with Gradient Descent
  - Variants of Gradient Descent
- **Linear Regression: Challenges and Solutions**
  - Linear Regression with Many Attributes
  - Dealing with Features of Different Scales
  - Dealing with Non-Linear Relationship
- Normal Equation

Linear Regression with Many Attributes

Bias (x_0)	Year (x_1)	# bedrooms (x_2)	# bathrooms (x_3)	Size (m²) (x_4)	Price ($) ($y$)
1	2016	4	2	113	560,000
1	1998	3	2	102	739,000
1	1997	3	0	100	430,000
1	2014	3	2	84	698,000
1	2016	3	0	112	688,888
1	1979	2	2	68	390,000
1	1969	2	1	53	250,000
1	1986	3	2	122	788,000
1	1985	3	3	150	680,000
1	2009	3	2	90	828,000

HDB prices from SRX

Notation:

- n = number of features
- $x^{(i)}$ = input features of the i-th training example
- $x_j^{(i)}$ = value of feature j in i-th training example

Hypothesis:

$$h_w(x) = w_0 x_0 + w_1 x_1 + w_2 x_2 + w_3 x_3 + w_4 x_4$$

Hypothesis (for n features):

$$h_w(x) = \sum_{j=0}^{n} w_j x_j = w^T x$$

vector

Weight Update (for n features):

$$w_j \leftarrow w_j - \gamma \frac{\partial J_{MSE}(w_0, w_1, \ldots, w_n)}{\partial w_j}$$

$$w_j \leftarrow w_j - \gamma \frac{1}{m} \sum_{i=1}^{m} \left(h_w(x^{(i)}) - y^{(i)}\right). x_j^{(i)}$$

Dealing with Features of Different Scales

x_0	x_1	x_2	x_3	x_4	y
Bias	Year	# bedrooms	# bathrooms	Size (m^2)	Price ($)
1	2016	4	2	113	560,000
1	1998	3	2	102	739,000
1	1997	3	0	100	430,000
1	2014	3	2	84	698,000
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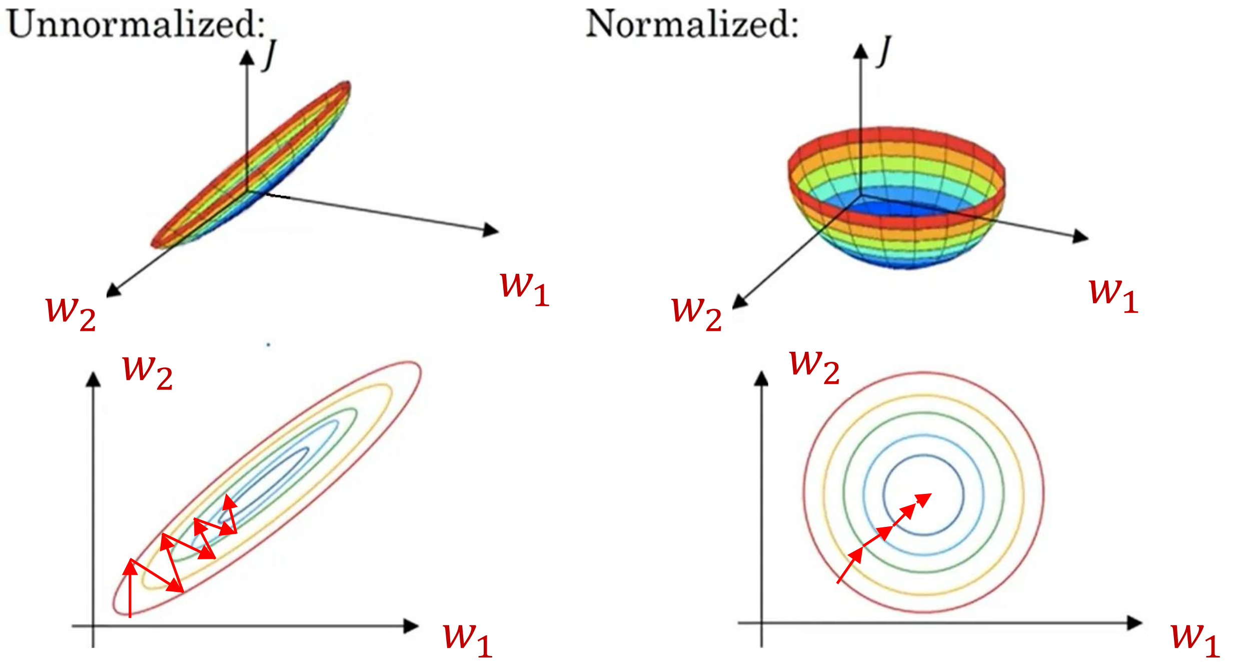
HDB prices from SRX



Each attribute has different scale:

$$1969 \le x_1 \le 2016$$

$$2 \le x_2 \le 5$$

$$0 \le x_3 \le 2$$

$$84 \le x_4 \le 150$$

Other methods of standardization also exists:
Min-max scaling, robust scaling, etc

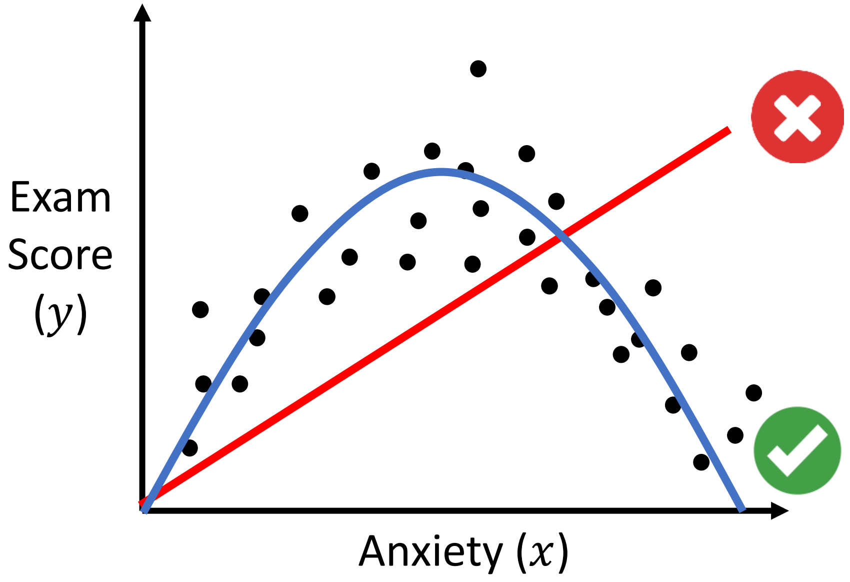
Mean normalization:

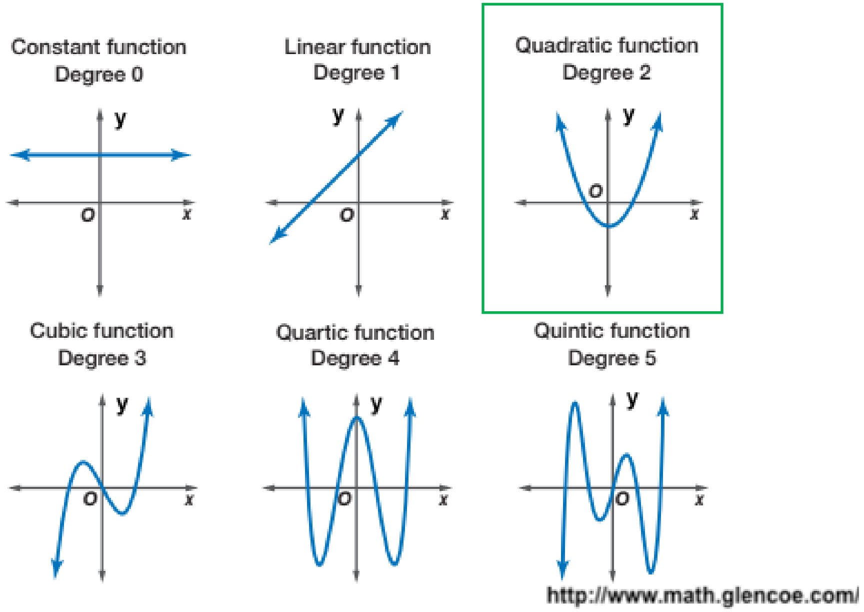
$$x_i \leftarrow \frac{x_i - \mu_i}{\sigma_i}$$

std dev

Image Credit: Andrew Ng

Dealing with Non-Linear Relationship





Which function?

$$h_w(x) = w_0 + w_1 x_1 + w_2 x_1^2$$

Polynomial Regression

Need to scale this!

Generally:

$$h_w(x) = w_0 + w_1 f_1 + w_2 f_2 + w_3 f_3 + \cdots + w_n f_n$$

Transformed features:

$e.g., f_1 = x_1, f_2 = x_1^2$

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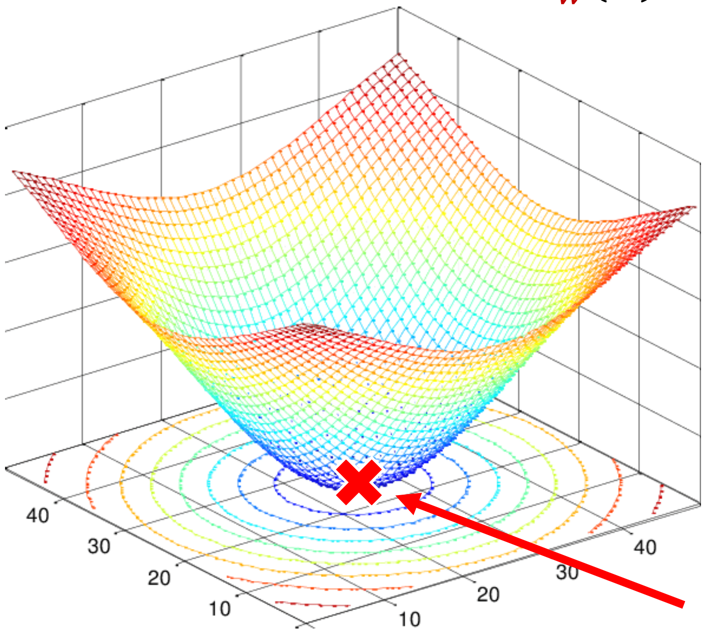
- **Normal Equation**

Normal Equation

$$X = \begin{bmatrix} 1 & x_1^{(1)} & & x_n^{(1)} \\ 1 & x_1^{(2)} & \dots & x_n^{(2)} \\ 1 & \vdots & & \vdots \\ 1 & x_1^{(m)} & & x_n^{(m)} \end{bmatrix} \quad w = \begin{bmatrix} w_0 \\ w_1 \\ \dots \\ w_n \end{bmatrix} \quad Y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \dots \\ y^{(m)} \end{bmatrix}$$

Bias

$$h_w(X) = Xw$$



Zero gradient!

Goal: find w that minimizes J_{MSE}:

Set $\dfrac{\partial J_{MSE}(w)}{\partial w} = 0$

A bunch of math…

$$2X^TXw - 2X^TY = 0$$

$$2X^TXw = 2X^TY$$

$$X^TXw = X^TY$$

$$\boxed{w = (X^TX)^{-1}X^TY}$$

Assume invertible

Gradient Descent vs Normal Equation

	Gradient Descent	**Normal Equation**
Need to choose γ	Yes	No
Iteration(s)	Many	None
Large number of samples n?	No problem	Slow, $(X^T X)^{-1} \rightarrow O(n^3)$
Feature scaling?	May be necessary	Not necessary
Constraints	-	$X^T X$ needs to be invertible

Summary

- Linear Regression: **fitting a line** to data
- Gradient Descent
  - Gradient Descent Algorithm: **follow –gradient** to reduce error
  - Linear Regression with Gradient Descent: **convex** optimization, **one minimum**
  - Variants of Gradient Descent: batch, mini-batch, stochastic
- Linear Regression: Challenges and Solutions
  - Linear Regression with Many Attributes: $h_w(x) = \sum_{j=0}^{n} w_j x_j = w^T x$
  - Dealing with Features of Different Scales: **normalize**!
  - Dealing with Non-Linear Relationship: **transform features**
- Normal Equation: **analytically** find the best parameters

Coming Up Next Week

- Logistic Regression
  - Gradient Descent
  - Multi-class classification
  - Non-linear decision boundary
- (More) Performance Measure
- (More) Model Evaluation

To Do

- **Lecture Training 5**
  - +100 Free EXP
  - +50 Early bird bonus
- **Problem Set 4**
  - Out today!