

# Chapter 3 Data Regression

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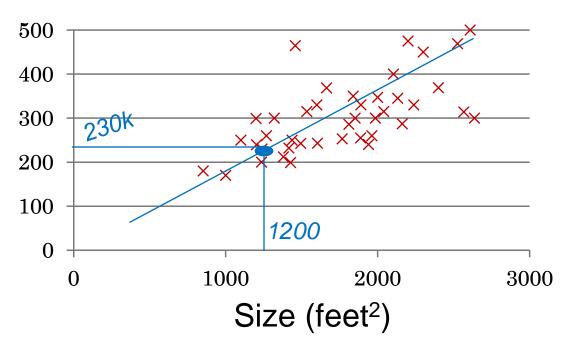
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- 3. Non-Linear regression
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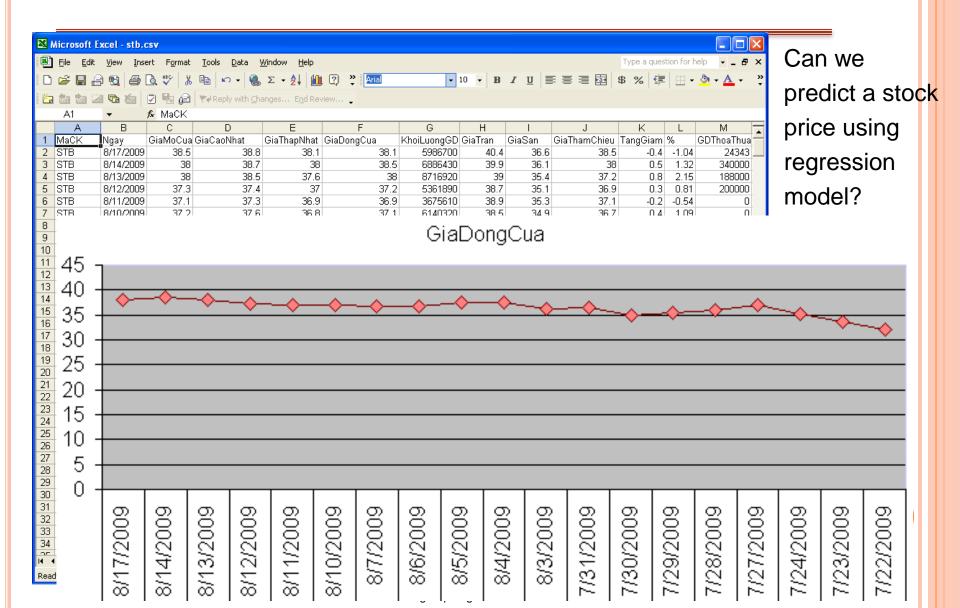
### REFERENCES

- [1] Jiawei Han, Micheline Kamber, and Jian Pei, "Data Mining: Concepts and Techniques", 3rd Edition, Morgan Kaufmann Publishers, 2012.
- [2] David Hand, Heikki Mannila, Padhraic Smyth, "Principles of Data Mining", MIT Press, 2001.
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- [4] Graham J. Williams, Simeon J. Simoff, "Data Mining: Theory, Methodology, Techniques, and Applications", Springer-Verlag, 2006.
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Price (\$1k)



- + Can we model the house price distribution based on their sizes?
- + Can we predict a house price based on its size?



The market basket analysis problem

→ Can we find out association rules between products in

tinned meat transactions? ice cream mozzarella coffee rice tomato sauce milk brioches ( frozen fish frozen vegetables juices beer crackers pasta yoghurt oil tunny coke water

biscuits

- Analyzing the factors that impact on the quality of e-banking services (based on surveys from users)
  - Easy to use (+0.209)
  - Fast response (+0.261)
  - The ability to link with other billing services (+0.199)
  - Feelings of individuality (+0.15)
  - Privacy and security issues (-0.25)
  - •

#### Regression

- J. Han et al (2001, 2006): Regression is a statistic mechanism that allows predicting real/numeric and continuous values
- Wiki (2009): Regression analysis is a statistic mechanism that allows estimating the correlation between independent variables
- R. D. Snee (1977): Regression is a statistic mechanism in data analytics and building models from experiments, it allows prediction, control, and learning the rules to which data is generated.
- Regression: Numeric data prediction (real-valued output)
- Classification: "prediction" for discrete values

- Regression model: Describe the relationship between a set of predictors/independent variables and one or some responses/dependent variables
- Regression equation

$$\mathbf{Y} = f(\mathbf{X}, \, \boldsymbol{\Theta})$$

**X**: a set of predictors/independent variables; describes the changes of responses/dependent variables Y

Y: responses/dependent variables; Describes the interesting facts/events

**θ**: Regression coefficients; Describes the relative effects of X on Y

#### Categories:

- Linear v.s nonlinear
  - ✓ Linear in parameters: Linear association between parameters that affect Y
  - Nonlinear in parameters: Non-linear association between parameters that affect Y
- Single variable v.s multiple variables
  - ✓ Single:  $X = (X_1)$  v.s. Multiple:  $X = (X_1, X_2, ..., X_k)$
- Parametric v.s nonparametric and semiparametric
- Symmetric v.s asymmetric
  - ✓ Symmetric: descriptive regression models (e.g., log-linear models)
  - ✓ Asymmetric: predictive regression models (e.g., generalized linear models)

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- o Parametric, nonparametric, and semiparametric
  - Parametric: regression models with finite parameters
  - Nonparametric: regression models with infinite parameters
  - Semiparametric: regression models with finite interesting parameters

Regression model	Description
Parametric	$Y = \theta_0 + \theta_1 * X$
Nonparametric	$Y = \theta_0 + f(X)$
Semiparametric	$Y = \theta_0 + \theta_1 * X_1 + f(X_2)$

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# 2. LINEAR REGRESSION

- Single variable (Univariate)
- Multiple variables (Multivariate)

#### Notations

- N: size of training examples
- x: input variable/feature
- ✓ y: output/target variable
- $(x^{(i)}, y^{(i)})$ :  $i^{th}$  learning sample
- $\checkmark (x^{(1)}, y^{(1)}) = (2100, 450)$

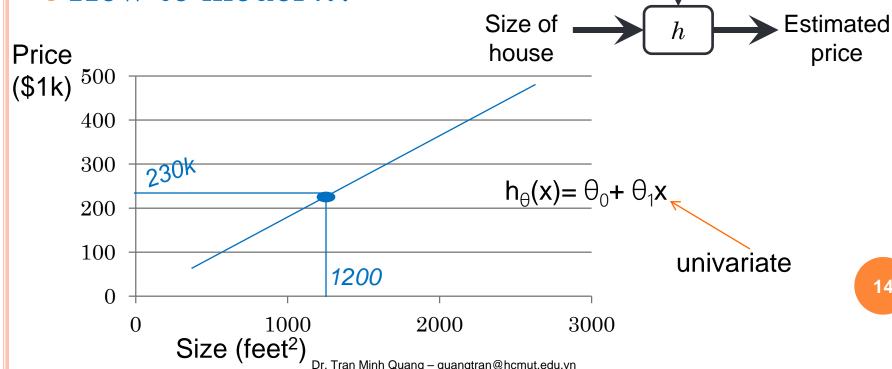
${f Size\ feet^2}$	Price (\$1k)
<b>(</b> x <b>)</b>	<b>(</b> y <b>)</b>
2100	450
1416	232
1534	315
852	178
• • •	• • •

Training Set

Learning Algorithm

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- Hypothesis (h)
- y = h(x); h is a mapping from x to y
- $\circ$  How to model h?



- Hypothesis (h):  $h_{\theta}(x) = \theta_0 + \theta_1 x =$  identify  $\theta_i$ ?
- Method: "try\_and\_error", evaluate the ability of the regression line in describing sample data.

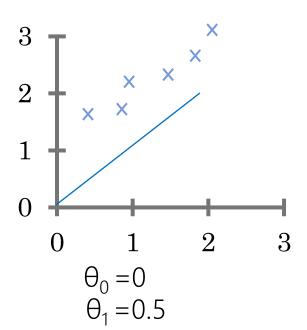
$$h_{\theta}(\mathbf{x}) = \theta_{0} + \theta_{1}\mathbf{x}$$

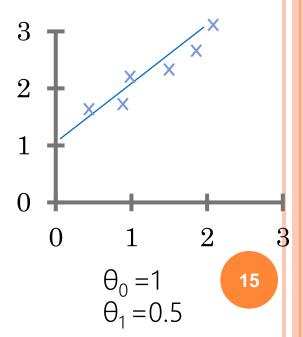
$$2 \quad \times \quad \times$$

$$1 \quad \times \quad \times$$

$$0 \quad 1 \quad 2 \quad 3$$

$$\theta_{0} = 2$$





- Chose  $(\theta_0, \theta_1)$  so that  $h_{\theta}(x^{(i)}) \simeq y^{(i)}$ ; i=1...N
  - o residual/prediction error

$$e = h_{\theta}(x^{(i)}) - y^{(i)}$$

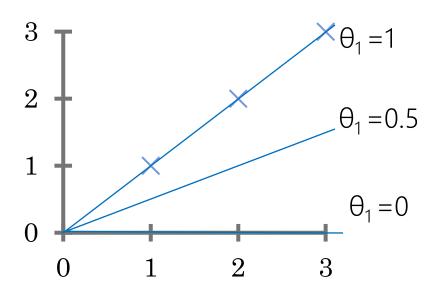
MSE

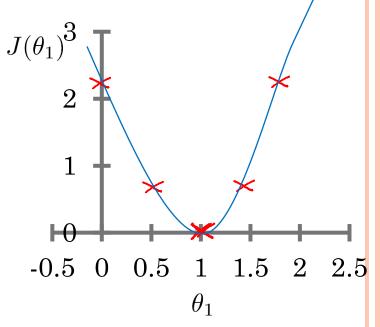
$$MSE = \frac{1}{N} \sum_{i=1}^{N} (h_{\theta}(x^{(i)}) - y^{(i)})^{2}$$

• Cost function  $J(\theta_0, \theta_1) => minimize$ 

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

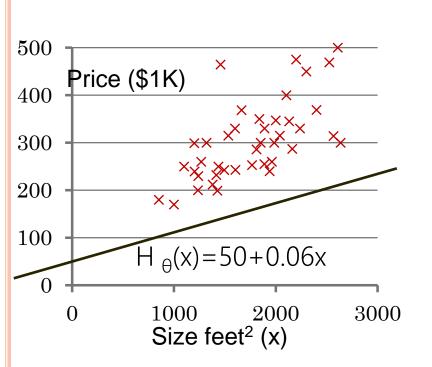
• Examine a simple case:  $\theta_0 = 0$ ,  $h_{\theta}(x) = \theta_1 x$ 

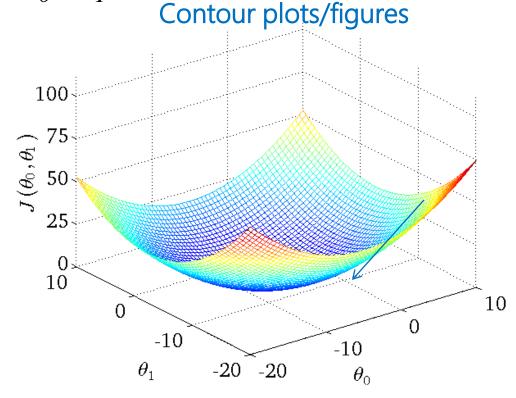




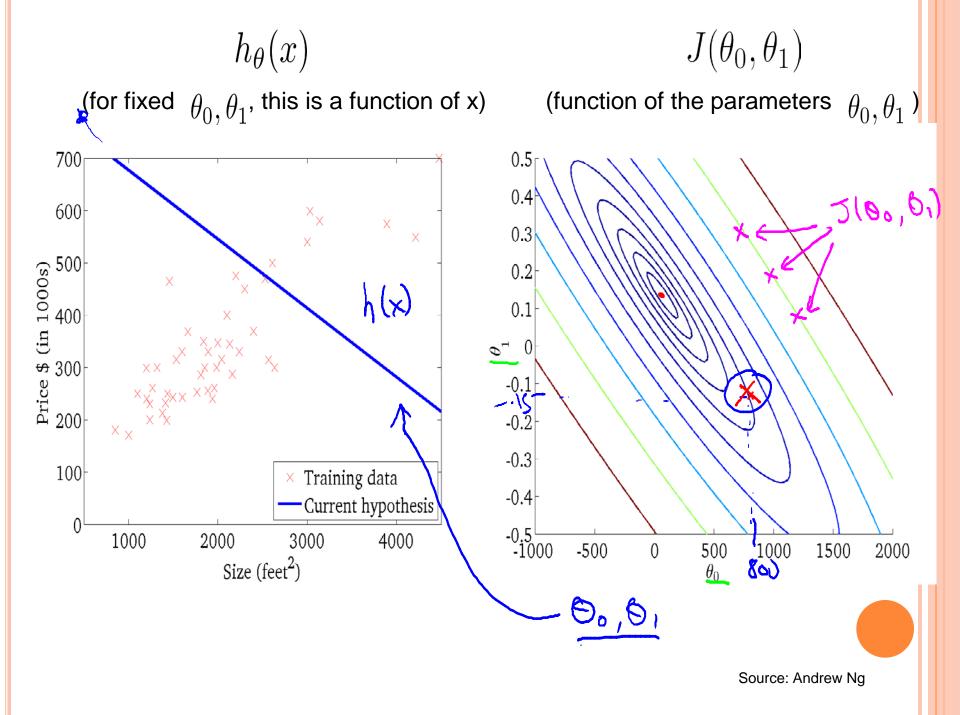
• 
$$\theta_{1} = 1 \Rightarrow J(\theta_{1}) = 0$$
;  $\theta_{1} = 0.5 \Rightarrow J(\theta_{1}) = 0.58$ ;  $\theta_{1} = 0 \Rightarrow J(\theta_{1}) = 2.3$ 

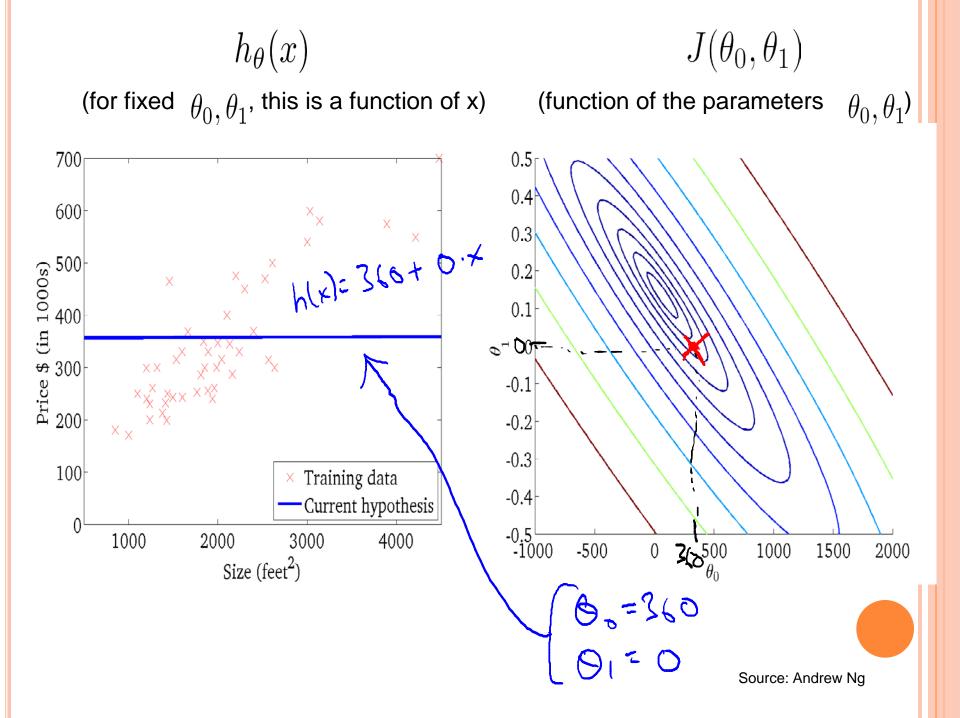
• An example with  $h_{\theta}(x) = \theta_0 + \theta_1 x$ 



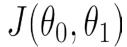


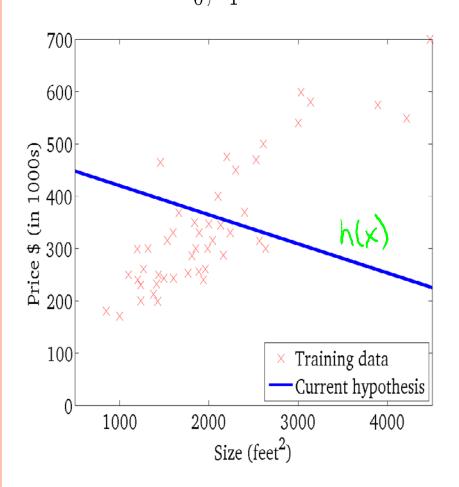
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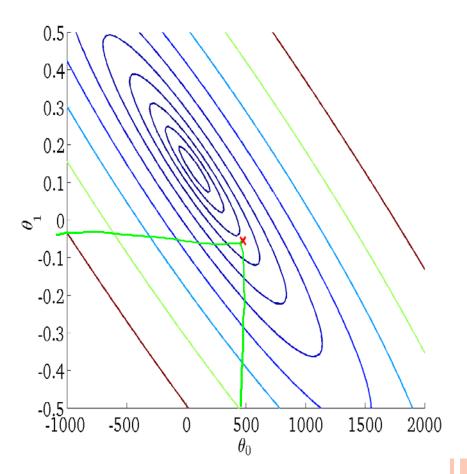




$$h_{\theta}(x)$$

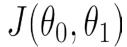


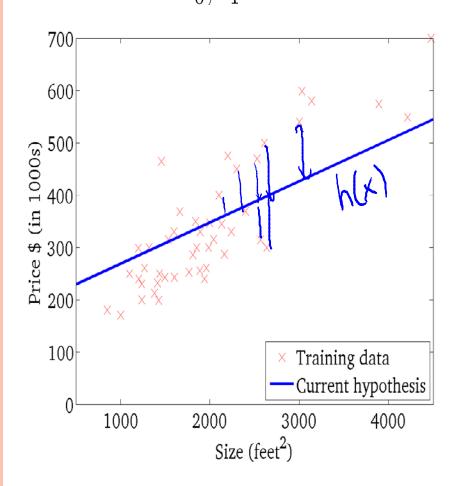


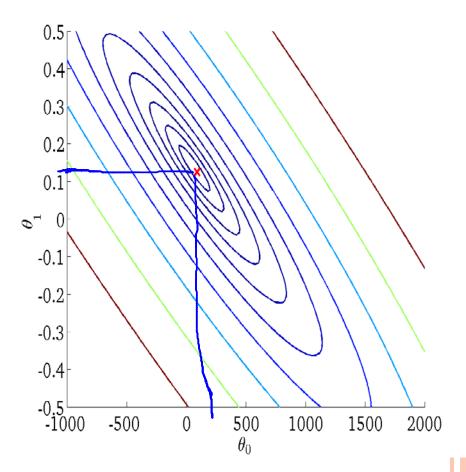




$$h_{\theta}(x)$$





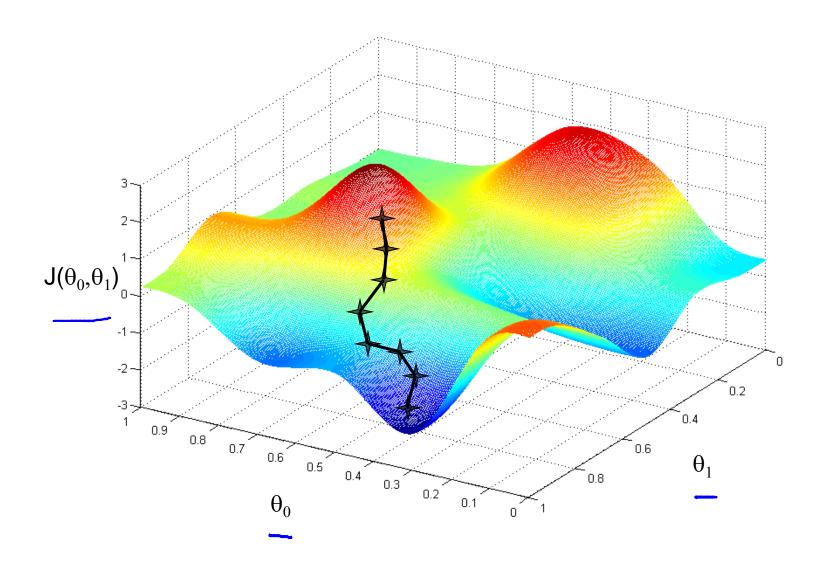


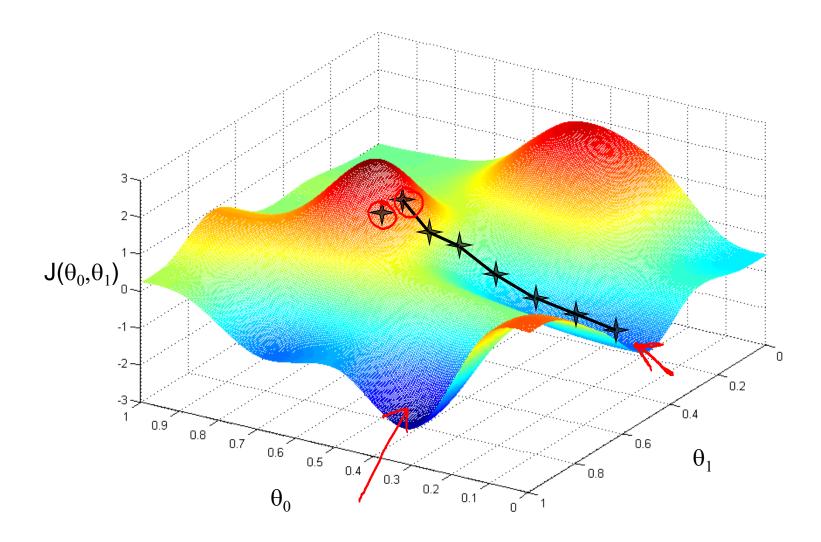


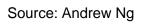
•Gradient descent method => find our the point that minimize  $J(\theta_0, \theta_1)$ 

#### •Method:

- Initiate with a random parameter  $(\theta_0, \theta_1)$ , ex.  $(\theta_0=0, \theta_1=0)$
- ii. Change  $(\theta_0, \theta_1)$  to reduce  $J(\theta_0, \theta_1)$
- iii. Iterate step ii until  $J(\theta_0, \theta_1)$  is (or we believe/accept that it is) minimum







#### Gradient descent algorithm

#### Repeat until convergence{

$$\theta_j = \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$$
 // for j=0 and j=1, simultaneously }
Learning rate

#### **Correct**: Simultaneously update

$$\begin{array}{ll} \operatorname{temp0} := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) & \operatorname{temp0} := \theta_0 \\ \operatorname{temp1} := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) & \theta_0 := \operatorname{temp0} \\ \theta_0 := \operatorname{temp0} & \operatorname{temp1} := \theta_1 \\ \theta_1 := \operatorname{temp1} & \theta_1 := \operatorname{temp1} \end{array}$$

#### Wrong:

$$temp0 := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1)$$

$$\theta_0 := temp0$$

$$temp1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1)$$

$$\theta_1 := temp1$$
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### UNIVARIATE LINEAR REGRESSION

• Gradient descent algorithm: minimize  $J(\theta_0, \theta_1)$ 

$$J(\theta_{0}, \theta_{1}) = \frac{1}{2N} \sum_{i=1}^{N} (h_{\theta}(x^{(i)}) - y^{(i)})^{2} \frac{\partial}{\partial \theta} J(\theta_{0}, \theta_{1})$$

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

$$\text{Repeat until convergence} \{$$

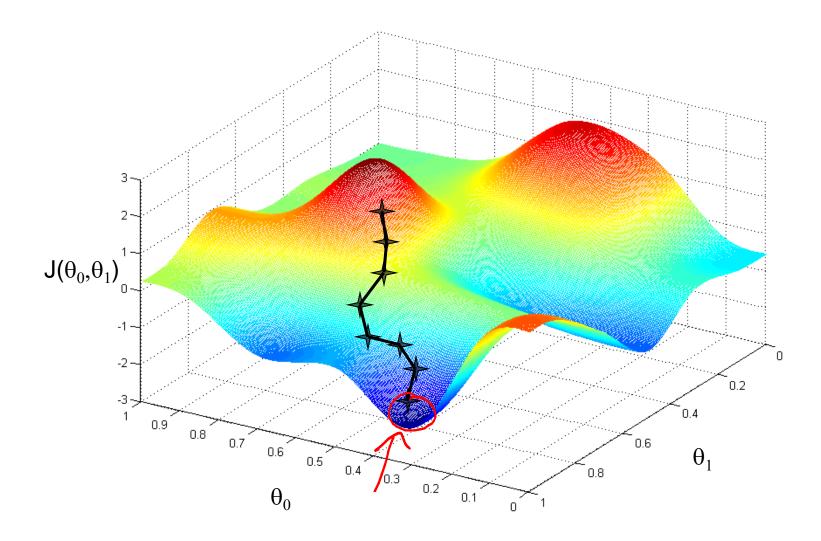
$$\theta_0 = \theta_0 - \alpha \frac{1}{N} \sum_{i=1}^{N} (h_{\theta}(x^{(i)}) - y^{(i)})$$

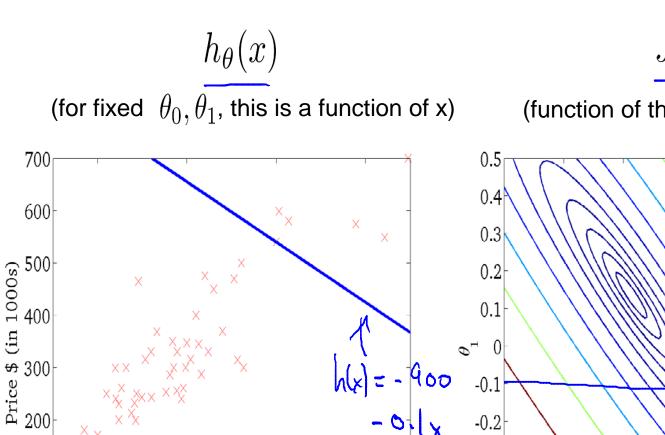
$$\theta_1 = \theta_1 - \alpha \frac{1}{N} \sum_{i=1}^{N} (h_{\theta}(x^{(i)}) - y^{(i)}) x^{(i)}$$

$$\frac{\partial}{\partial \theta_1} J(\theta_0,\theta_1)$$

$$Update \ \theta_0 \ and \ \theta_1 \ simultaneously$$

$$\}$$

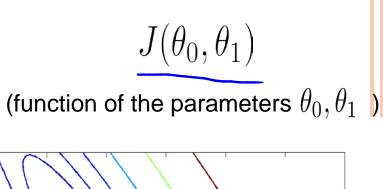


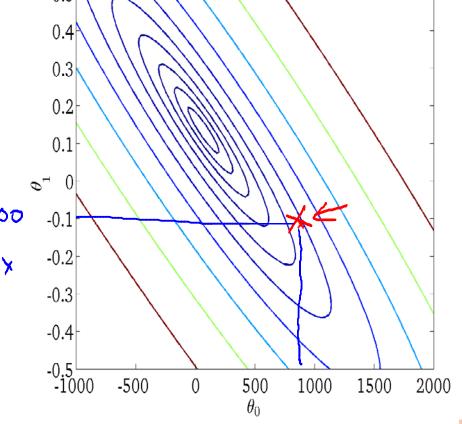


× Training data

Current hypothesis

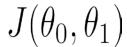
Size (feet<sup>2</sup>)



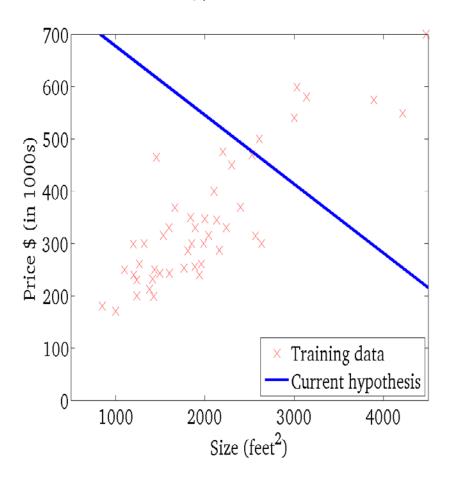


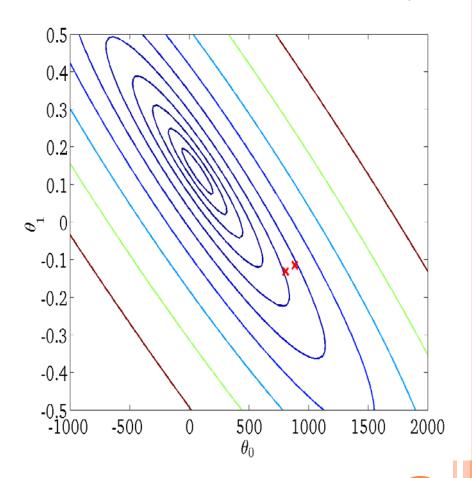


$$h_{\theta}(x)$$



(function of the parameters  $\; heta_0, heta_1 \; )$ 



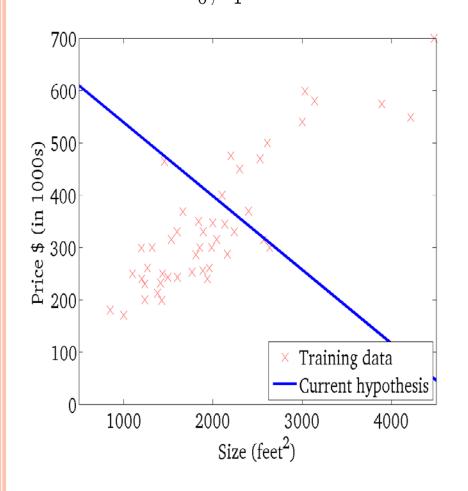


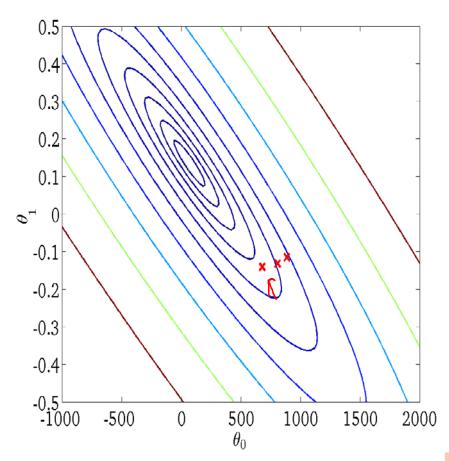


$$h_{\theta}(x)$$



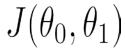
(function of the parameters  $\; heta_0, heta_1 \;$ )

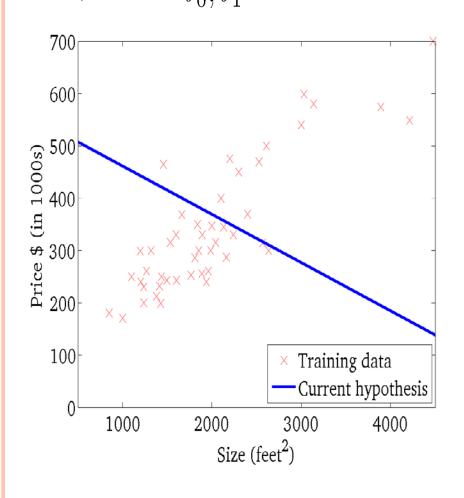


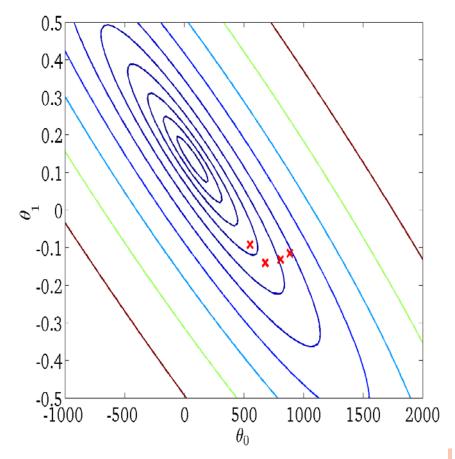




$$h_{\theta}(x)$$

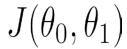


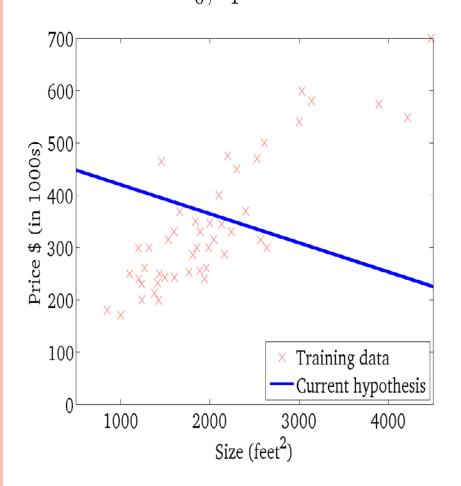


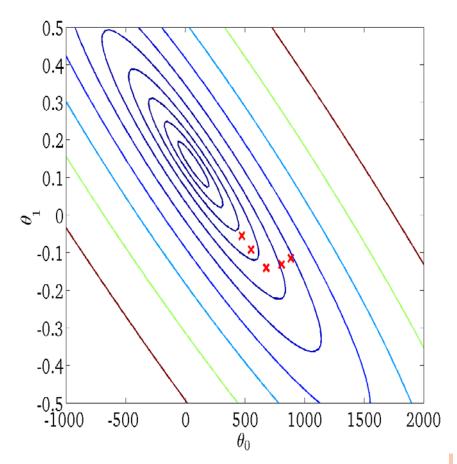




$$h_{\theta}(x)$$

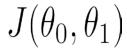


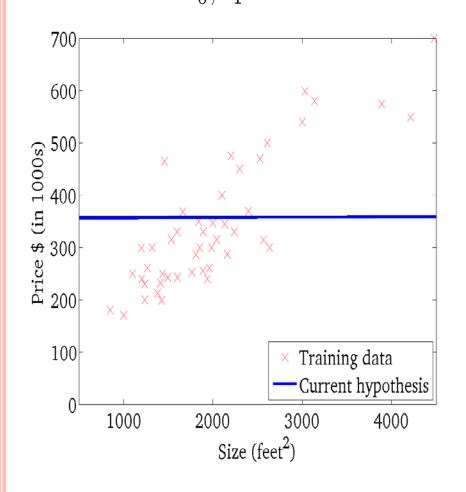


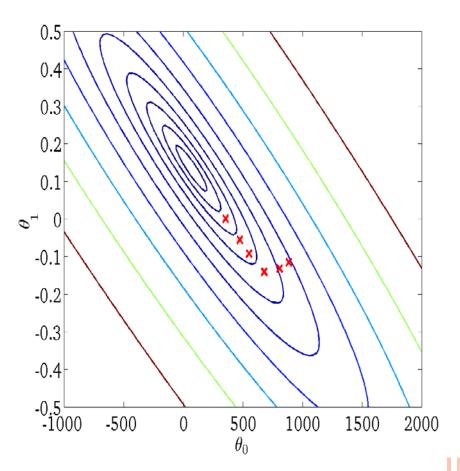




$$h_{\theta}(x)$$

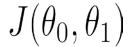


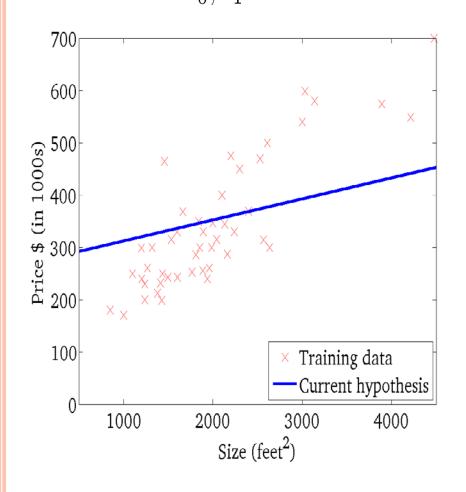


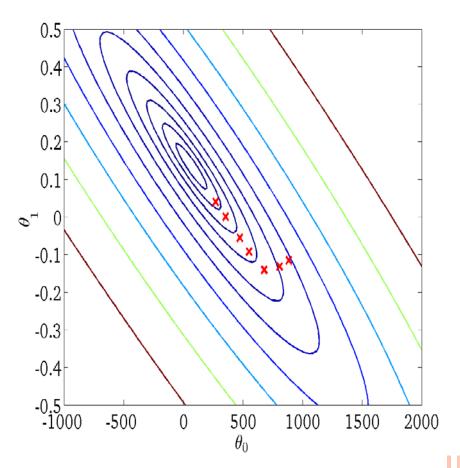




$$h_{\theta}(x)$$

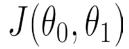


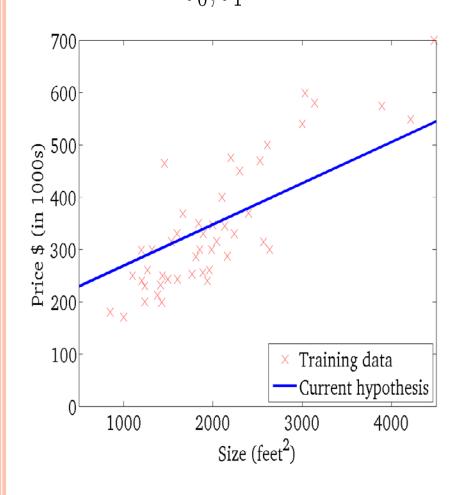


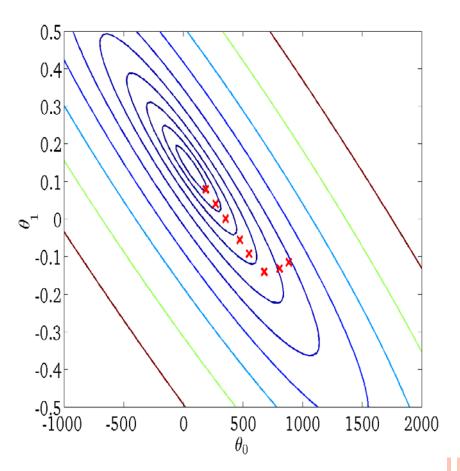




$$h_{\theta}(x)$$



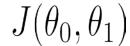




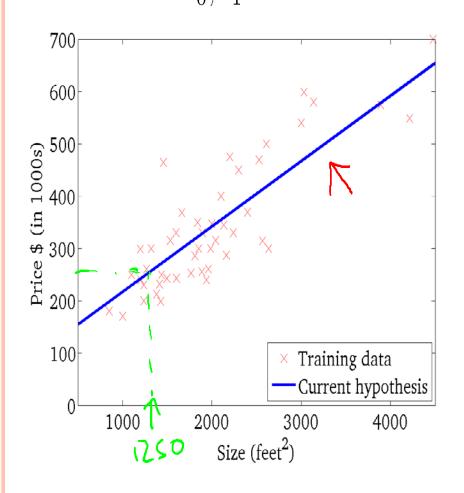


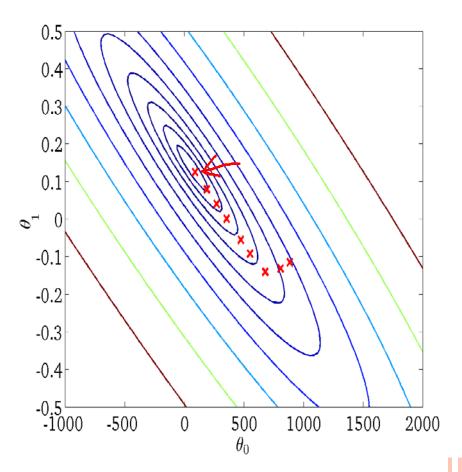
$$h_{\theta}(x)$$

(for fixed  $\theta_0, \theta_1$ , this is a function of x)



(function of the parameters  $\theta_0, \theta_1$ 





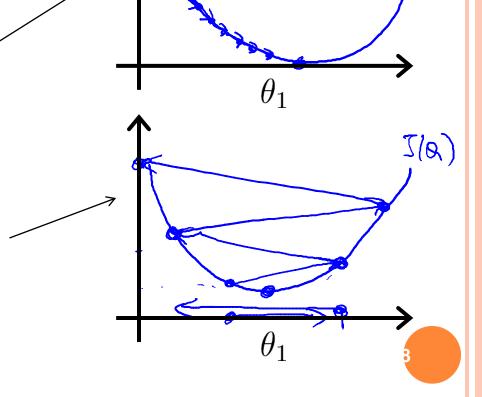


• Learning rate α

$$\theta_1 = \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)$$

✓ Too small: Learn slowly

✓ Too big: Difficult to converge to the point where  $J(\theta_0, \theta_1)$  is minimum



J(0,)

- o Summary: Given N samples, a univariate regression model is described as follow (e, describes the change of Y which is not explainable from X)
  - Straight line form

$$y_i = h_\theta(x_i) = \theta_0 + \theta_1 x_i + e_i, i = 1, 2, ..., N$$

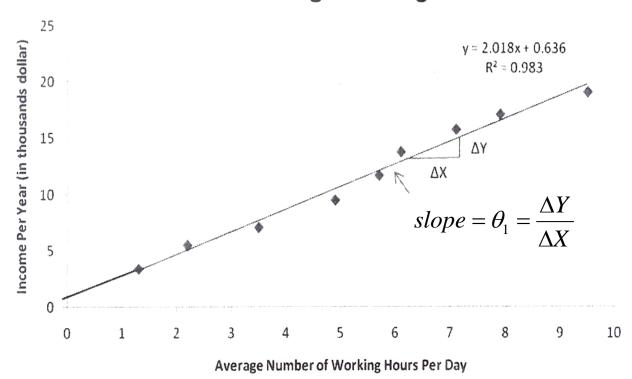
Parabol form

$$y_i = h_\theta(x_i) = \theta_0 + \theta_1 x_i + \theta_2 x_i^2 + e_i, i = 1, 2, ..., N$$

• Estimating  $(\theta_0, \theta_1)$  by gradient descent method or can be quickly estimated by:

$$\theta_1 = \frac{\sum_{i=1}^{N} (x^{(i)} - \overline{x})(y^{(i)} - \overline{y})}{\sum_{i=1}^{N} (x^{(i)} - \overline{x})^2} \qquad \theta_0 = y - \theta_1 x$$

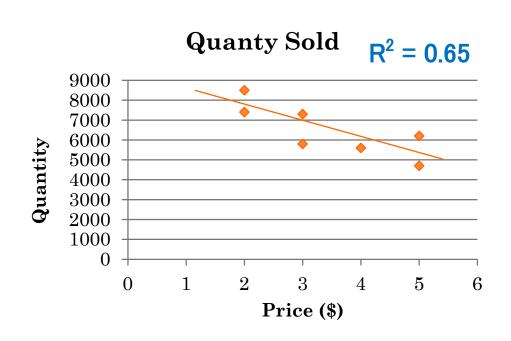
#### **Income vs Average Working Hours**



$$\bullet Y = \theta_0 + \theta_1^* X1 \rightarrow Y = 0.636 + 2.018^* X$$

•The sign of  $\theta_1$  describes the effect direction (positive/negative) of X on Y.

Quantity Sold	Price(\$)
8500	2
4700	5
5800	
7400	2
6200	5
7300	
5600	4



y=quantySold=9323-823\*price

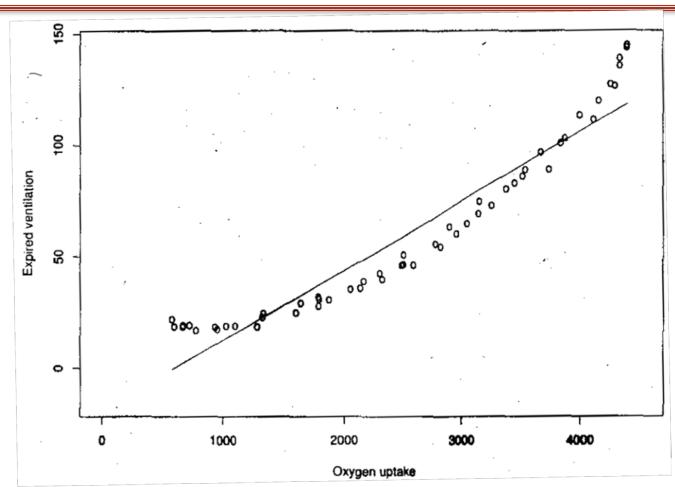


Figure 11.1, [2], pp. 372. Expired ventilation plotted against oxygen uptake in a series of trials, with fitted straight line:  $y = \theta_0 + \theta_1 x$ .

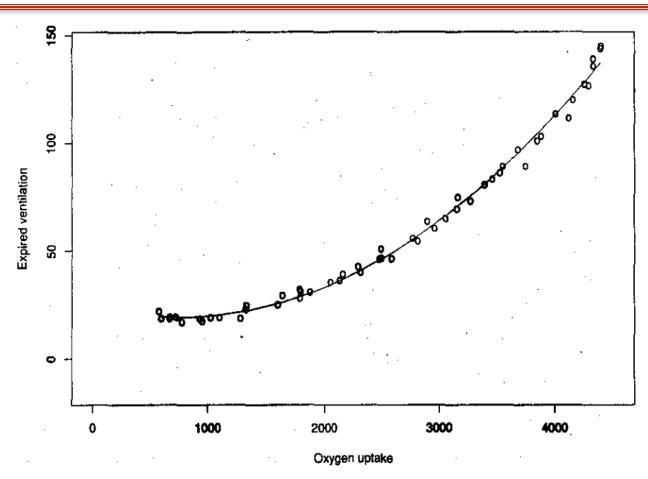


Figure 11.2, [2], pp. 373. The data from Figure 11.1 with a model that includes a term in  $x^2$ :  $y = \theta_0 + \theta_1 x + \theta_2 x^2$ .

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• The house prices is affected by several variables/factors

	Number of			
$Size (feet^2)$	rooms	${f Floors}$	$\mathbf{Age}$	Price(\$1K)
2104	5	1	45	460
1416	3	2	40	232
1534	3	2	30	315
852	2	1	36	178
•••	•••	• • •	• • •	• • •

n: number of input attributes (e.g., n = 4)

x<sup>(i)</sup>: input (features) of the i<sup>th</sup> training sample

x<sub>i</sub>(i): value of attribute j in the training sample i<sup>th</sup>

y<sup>(i)</sup>: i<sup>th</sup> output in the training dataset

E.x., 
$$x^{(1)} = \begin{bmatrix} 2014 \\ 5 \\ 1 \\ 45 \end{bmatrix}; x_3^{(1)} = 1$$

ΛΛ

### • Hypothesis:

$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \dots + \theta_n x_n$$

$$h_{\theta}(x) = 100 + 3x_1 + 2x_2 + 1.5x_3 - 2x_4$$

• Presenting in a matrix form  $(x_0=1)$ 

$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}; \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}; \theta^T = [\theta_0, \theta_1, \theta_2, \dots, \theta_n]$$

$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \dots + \theta_n x_n = \theta^T x$$

• Gradient descent:

$$h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \dots + \theta_n x_n = \theta^T x$$

- Coefficients  $\theta(\theta_0, ..., \theta_n)$ : an n+1 vector
- Minimize:  $J(\theta) = J(\theta_0, ..., \theta_n)$

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

### Repeat until convergence{

$$\theta_j \coloneqq \theta_j - \alpha \frac{\partial}{\partial \theta_i} J(\theta)$$
 // simultaneously update for every j=0,...,n

## 2.2. Hồi Qui Tuyến Tính Đa Biến

### Repeat until convergence{

$$\theta_j \coloneqq \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \text{ // simultaneously update for every j=0,...,n}$$

$$\theta_0 = \theta_0 - \alpha \frac{1}{N} \sum_{i=1}^{N} (h_{\theta}(x^{(i)}) - y^{(i)}) x_0^{(i)} x_0^{(i)} = 1$$

$$\theta_1 = \theta_1 - \alpha \frac{1}{N} \sum_{i=1}^{N} (h_{\theta}(x^{(i)}) - y^{(i)}) x_1^{(i)}$$

$$\theta_2 = \theta_2 - \alpha \frac{1}{N} \sum_{i=1}^{N} (h_{\theta}(x^{(i)}) - y^{(i)}) x_2^{(i)}$$

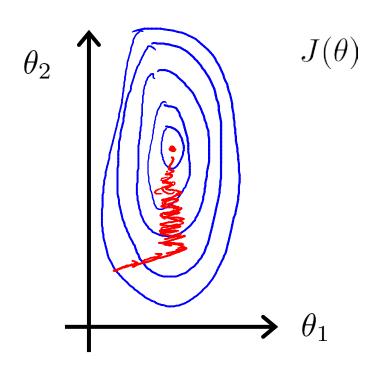
....

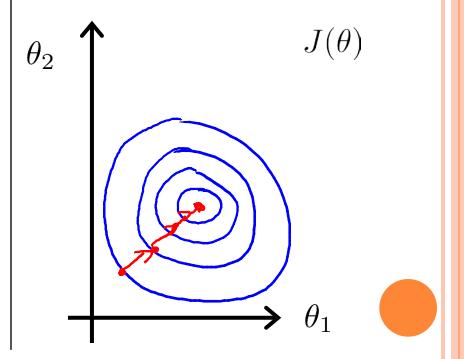
- Feature scaling: to assure that all input features are in the same scale
  - E.g.,  $x_1 = \text{size } (0 2000 \text{ feet}^2)$  $x_2 = \text{number of rooms } (1 - 5)$ 
    - => They are not in the same scale. The convergence speed is affected because of this imbalance scaling.

• Assure that features are in the same scale

E.g.  $x_1 = \text{size } (0-2000 \text{ feet}^2)$  $x_2 = \text{number of bedrooms } (1-5)$  Scaled:  $x_1 = size/2000$ 

 $x_2$ = number of bedrooms /5





Source: Andrew Ng

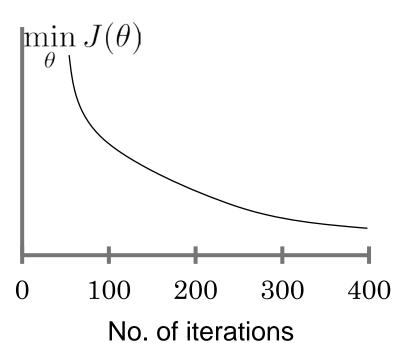
- Feature scaling
  - Normalize all feature to a range of [-1, 1]
  - Ex.,  $x_0 = 1$ ;  $0 \le x_1 \le 3$ ;  $-2 \le x_2 \le 0.5 => \mathbf{OK}$ -100  $\le x_3 \le 100$ ;  $-0.0001 \le x_4 \le 0.0001 => \mathbf{Normalize}$

- Apply normalization methods in chapter 2
  - Ex.

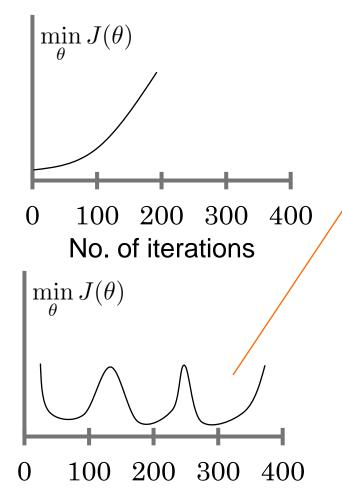
$$v' = \frac{v - v}{\sigma v}$$

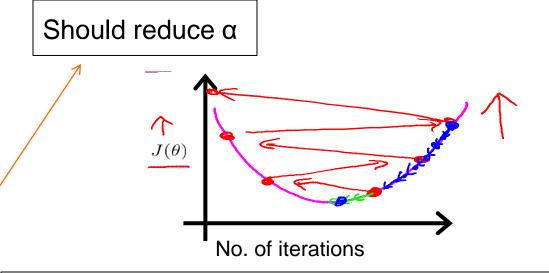
$$v' = \frac{v - \overline{v}}{V_{\text{max}} - V_{\text{min}}}$$

- Validate the Gradient descent algorithm
  - $J(\theta)$  must decrease after each iteration
  - We can plot  $J(\theta)$  by  $\theta$  for intuitively check the convergence ability of the algorithm



### • Un-converged gradient descent





-α too small: slow convergence

-α too large:  $J(\theta)$  may not reduce at each

iteration => the algorithm may no converge

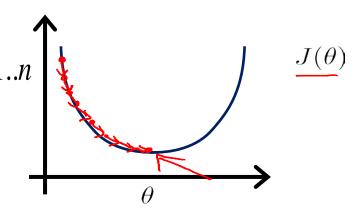
- **try** α: 0.001, 0.003, 0.01, 0.03, 0.1, 0.3,...

 $\circ$  Use normal equation to identify  $\theta$ 

#### **Gradient Descent**

$$\frac{\partial}{\partial \theta_{j}} J(\theta) = \frac{1}{N} \sum_{i=1}^{N} (h_{\theta}(x^{(i)}) - y^{(i)}) x_{j}^{(i)} = 0; \forall j = 1..n$$

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



Examples: N = 4, X: an Nx(n+1) matrix; y: an Nx1 matrix

	size (feet²)	No. of rooms	Floors	Years	Price (\$1K)
$\underline{} x_0$	$x_1$	$x_2$	$x_3$	$x_4$	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

$$X = \begin{bmatrix} 1 & 2104 & 5 & 1 & 45 \\ 1 & 1416 & 3 & 2 & 40 \\ 1 & 1534 & 3 & 2 & 30 \\ 1 & 852 & 2 & 1 & 36 \end{bmatrix}$$

$$y = \begin{bmatrix} 460 \\ 232 \\ 315 \\ 178 \end{bmatrix}$$

$$\theta = \left(\mathbf{X}^T \mathbf{X}\right)^{-1} \mathbf{X}^T \mathbf{Y}$$

• Given a training dataset: N examples, n features

#### <u>Gradient descent</u>

- must select α
- needs a large number of iterations
- workable event with a large n (e.g., n = 10<sup>6</sup>)

#### Normal equation

- don't need to select α
- don't need iterations
- Must compute (X<sup>T</sup>X)<sup>-1</sup>
- May not work when n is large (when n = 10<sup>4</sup> then gradient descent should be used)

o Note: the non-invertible issue in the normal equation method, i.e.,  $(X^TX)$  is not invertible

#### • Resolve:

- Check the linear dependence of variables. Ex., the size in meter  $(x_1)$  and the size in feet  $(x_2) => remove$  dependent variables
- Too much features (n > N). Ex., n = 20, N = 10 => reduce the number of features; find surrogate features; correct more data samples,...

### • Another example:

Quantity Sold	Price(\$)	Advertising (\$)
8500	2	2800
4700	5	200
5800	3	400
7400	2	500
6200	5	3200
7300	3	1800
5600	4	900

#### SUMMARY OUTPUT

Regression	Statistics
Multiple R	0.980681
R Square	0.96174
Adjusted R Square	0.942604
0	040 5000

Standard Error 310.5239

Observations 7

y = Quantity Sold = 8536.214 -835.722 \* Price + 0.592 \* Advertising

#### **ANOVA**

	df	SS	MS	F	Significance F
Regression	2	9694300	4847150	50.26854	0.0014641
Residual		385700.4	96425.11		
Total	6	10080000			

		Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	8536.21	386.9117	22.06243	2.5E-05	7461.974654	9610.453	7461.975	961 <mark>0.453</mark>
Price(\$)	-835.72	99.65304	-8.38632	0.001106	-1112.40356	-559.041	-1112.4	-559.041
Advertising (\$)	0.59223	0.104347	5.675579	0.004755	0.302515325	0.881942	0.302515	0.881942

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# 3. Non-linear regression

## $\mathbf{o} \mathbf{Y} = \mathbf{f}(\mathbf{X}, \boldsymbol{\theta})$

- Y is a non-linear function in terms of relationship between parameters  $\theta$ .
- Ex: Exponential, logarithmic function, Gauss, ...

$$f(x,\theta) = \frac{\theta_1 x}{\theta_2 + x}$$

- $\circ$  Identify optimal  $\theta$ : Optimization algorithms
  - Local optimization
  - Global optimization (using sum of squared residuals/errors)

## 4. APPLICATIONS

- Data mining
  - Data preprocessing: Smoothing, noise removal,...
  - Mining tasks: numerical-values prediction, descriptive analysis
- Apply in many domains: biology, agriculture, social issues, economy, business, finances, insurance, e-commerce, marketing, security, science, robotics, control systems, automation,...

- Assumptions
  - Data distribution: the relationship between predictors and dependent variables
  - Independence of predictors
  - Continuous values of variables (both predictor & responses)
  - Errors: How to identify them?
- The amount of data processed is not large
- How to identify the regression model
- Advanced techniques for regression:
  - Artificial Neural Network (ANN)
  - Support Vector Machine (SVM)

- Evaluation of a regression model:
  - Collect new data to evaluate the prediction results
  - Use the existing data (as testing dataset) for evaluation
  - Data splitting
    - Training data: To build the model
    - ✓ Testing data → validate/evaluate the model
  - K-fold cross-validation
    - ✓ Iterate k times:
      - ✓ Training data: (k-1) portions of data
      - ✓ Test data: the  $k^{th}$  portion of data → accuracy
    - ✓ Average(accuracy) of k times

- Evaluation of the regession model:
  - Accuracy
    - ✓ Sum of squared errors (SSE)
    - -> Overall measure of errors: smaller is better

$$SSE = \sum_{i=1}^{n} (y_i - y_i)^2$$

✓ Mean squared error (MSE): measure of the variability in the response variable left unexplained by the regression: **smaller is better** 

$$MSE = \frac{SSE}{n-m-1}$$

(n: sample size, m: number of regression coefficients)

- OAccuracy (Con't)
  - ✓ The standard error of the estimate (S)
  - ✓ Đánh giá sai số thông thường trong quá trình dự đoán, sự sai lệch giữa giá trị dự đoán và giá trị thực của biến đáp ứng
  - ✓ Measure the common error in the prediction process. It is the mean difference between the predicted and the actual values.
  - ✓ Presents the precision of the prediction generated by the regression model \_\_\_\_\_

$$S = \sqrt{MSE} = \sqrt{\frac{SSE}{n - m - 1}}$$

- Factors affect the success of building regression models
  - ✓ Proper problem formulation
  - Selection of important variables and model form
  - ✓ Good dataset (both in volume and quality)
  - ✓ The use of good coefficient estimation procedures (e.g., gradient descent)
  - ✓ Model validation techniques

## 6. SUMMARY

### Regression

- A statistical technique, applied to continuous attributes/features
- Simple yet useful, applicable in various domains
- One of example showing the contribution of statistics in data mining
- Types: Linear/non-linear, Univariate/Multivariate, Parametric/Non-parametric/Semi-parametric,
   Symmetric/Assymetric



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