DS 4400

Machine Learning and Data Mining I

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Announcements

- HW 1
  - Is due on Monday, Sept. 28
- Python tutorials
  - Panda data frames tutorial by Alex Wang
    - Wed, Sept. 23, 5-6pm
  - Same Zoom link as office hours
  - Recording of first tutorial is available on Canvas under “Lecture Recording”

Outline

- Linear regression
- Simple linear regression
  - MSE as loss function
  - Derivation of optimal solution
  - Correlation coefficient, covariance, and connection to regression
  - Example of linear regression fit
  - Lab in Python
- Multiple linear regression

Linear regression

Supervised Learning: Regression

Training

Data → Pre-processing → Feature extraction → Learning model

Labeled

$x_i, y_i \in R$

Normalization

Feature Selection

Regression

$f(x)$

Testing

New data → Learning model → Predictions

$y' = f(x') \in R$

Unlabeled

x'

$f(x)$

Response variable

Regression

Steps to Learning Process

- Define problem space
- Collect data
- Extract feature
- Pick a model (hypothesis)
- Develop a learning algorithm
  - Train and learn model parameters
- Make predictions on new data
  - Testing phase
- In practice, usually re-train when new data is available and use feedback from deployment

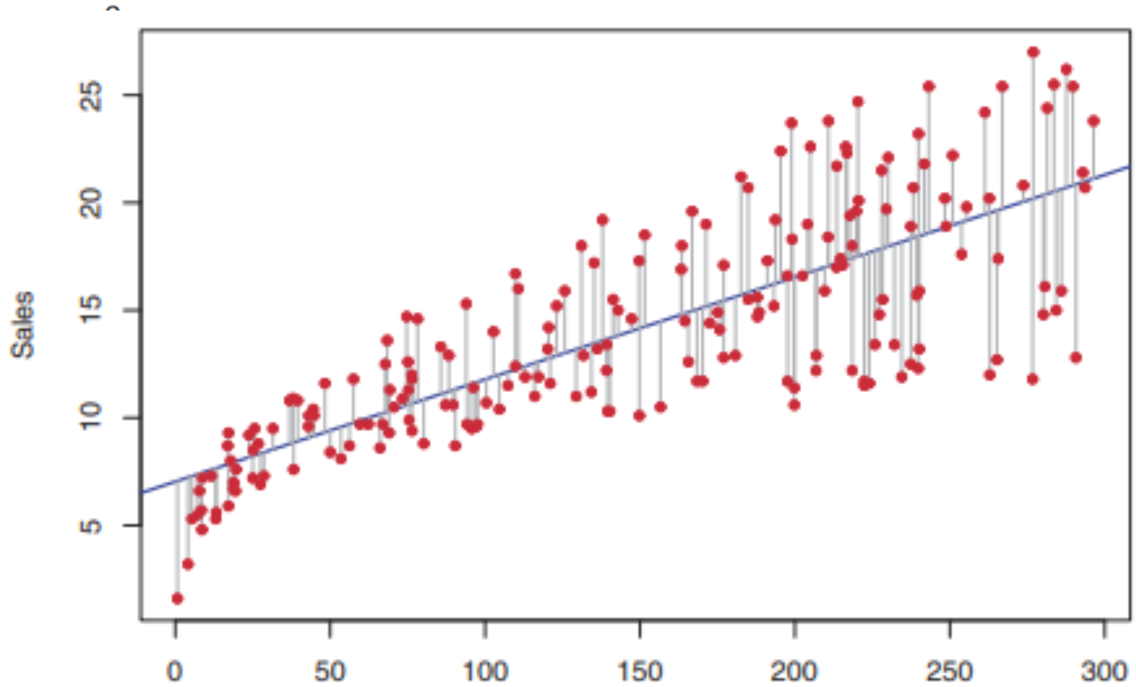
Linear regression

- One of the most widely used techniques
- Fundamental to many complex models
  - Generalized Linear Models
  - Logistic regression
  - Neural networks
  - Deep learning
- Easy to understand and interpret
- Efficient to solve in closed form
- Efficient practical algorithm (gradient descent)

Linear regression

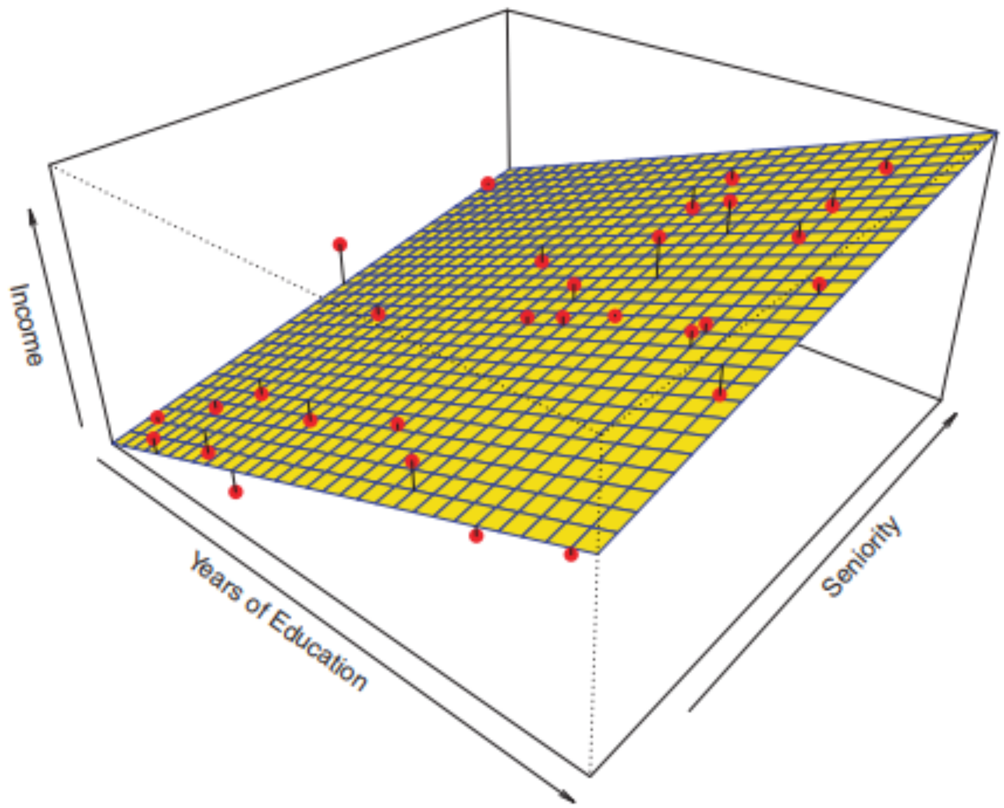
Given:

- Data $X = \{x_1, \ldots x_N\}$, where $x_i \in R^d$ — Features
- Corresponding labels $Y = \{y_1, \ldots y_N\}$, where $y_i \in R$ — Response variables



Simple Linear Regression: 1 predictor

Income Prediction



Linear Regression with 2 predictors

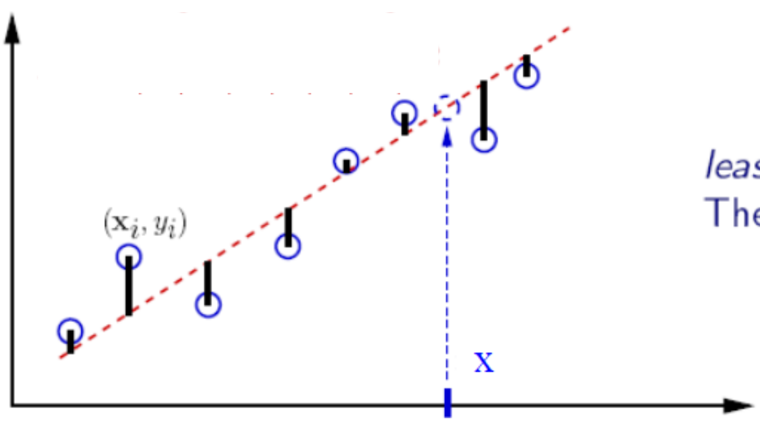
Multiple Linear Regression

Hypothesis: linear model

- Hypothesis: $h_\theta(x) = \theta_0 + \theta_1 x$

Simple linear regression
Regression model is a line with 2 parameters: θ_0, θ_1

- Fit model by minimizing sum of squared errors



least squares (LSQ)
The fitted line is used as a predictor

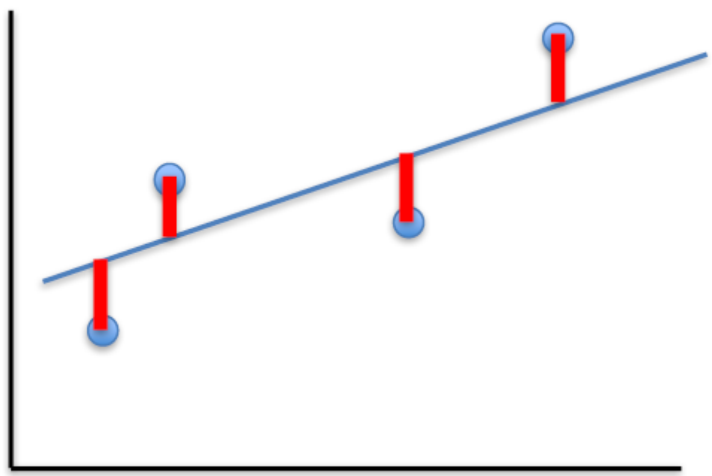
Least-Squares Linear Regression

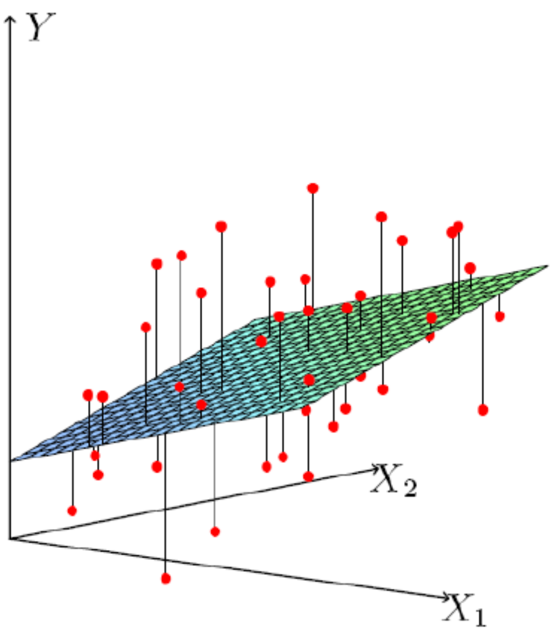
- Cost Function

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N}[h_\theta(x_i) - y_i]^2$$

Mean Square Error (MSE)

- Fit by solving $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

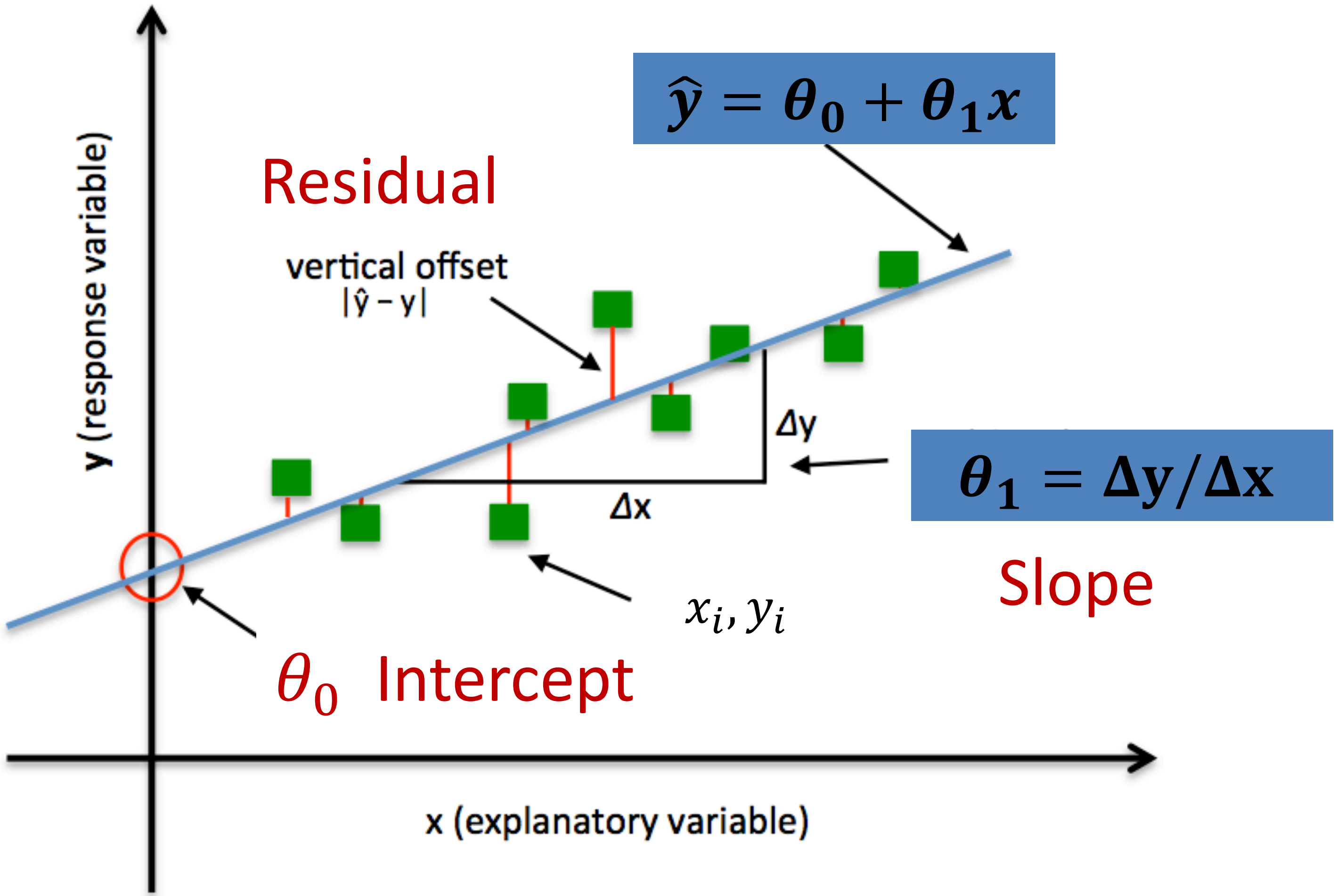




Terminology and Metrics

- Residuals
  - Difference between predicted values and actual values
  - Predicted value for example i is: $\widehat{y}_i = h_\theta(x_i)$
  - $R_i = \left|y_i - \widehat{y}_i\right| = |y_i - (\theta_0 + \theta_1 x_i)|$
- Residual Sum of Squares (RSS)
  - $RSS = \sum {R_i}^2 = \sum \left[y_i - (\theta_0 + \theta_1 x_i)\right]^2$
- Mean Square Error (MSE)
  - $MSE = \frac{1}{N} \sum R_i^2 = \frac{1}{\mathrm{N}} \sum \left[y_i - (\theta_0 + \theta_1 x_i)\right]^2$

Interpretation



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

MSE$= \frac{1}{N}\sum_{i=1}^{N}[h_\theta(x_i) - y_i]^2$

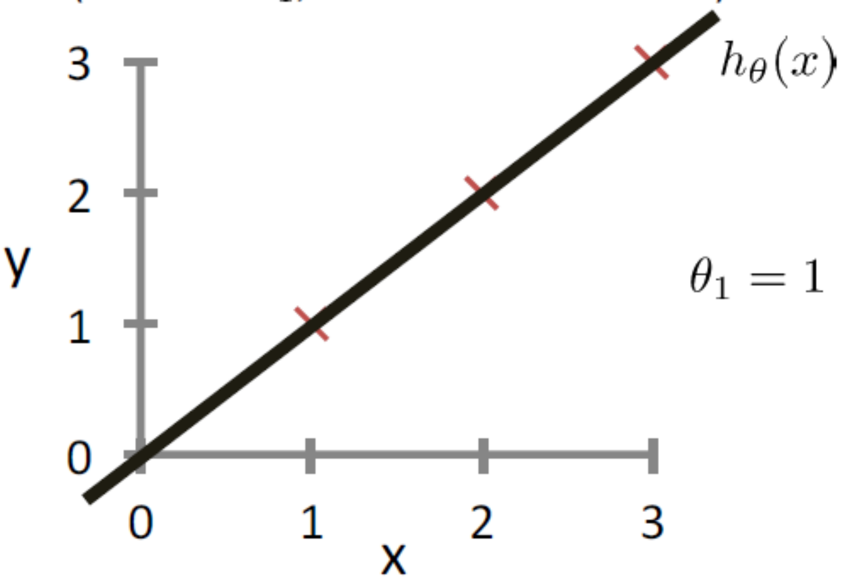
Intuition on MSE

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N}[h_\theta(x_i) - y_i]^2$$

For insight on J(), let's assume $x \in \mathbb{R}$ so $\boldsymbol{\theta} = [\theta_0, \theta_1]$

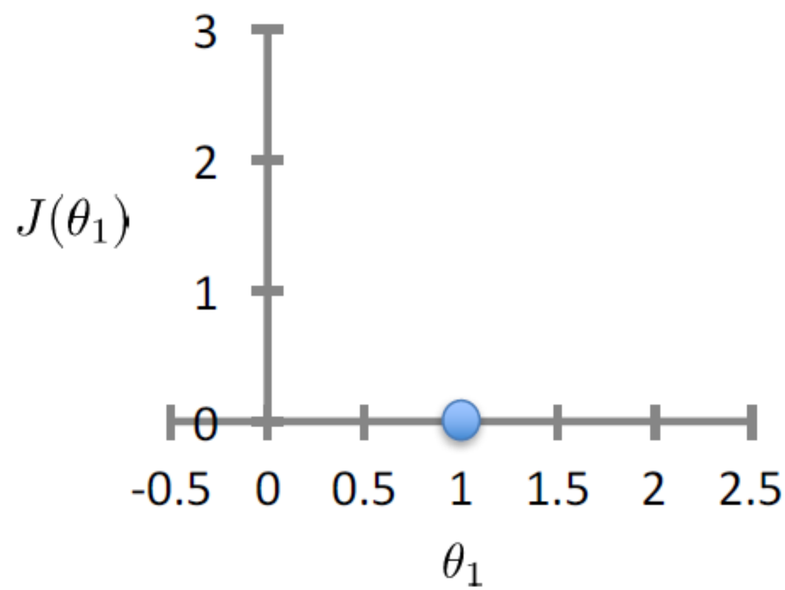
$h_\theta(x)$

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



$J(\theta_1)$

(function of the parameter θ_1)



Fix θ_0 =0

Intuition on MSE

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N}[h_\theta(x_i) - y_i]^2$$

For insight on J(), let's assume $x \in \mathbb{R}$ so $\boldsymbol{\theta} = [\theta_0, \theta_1]$

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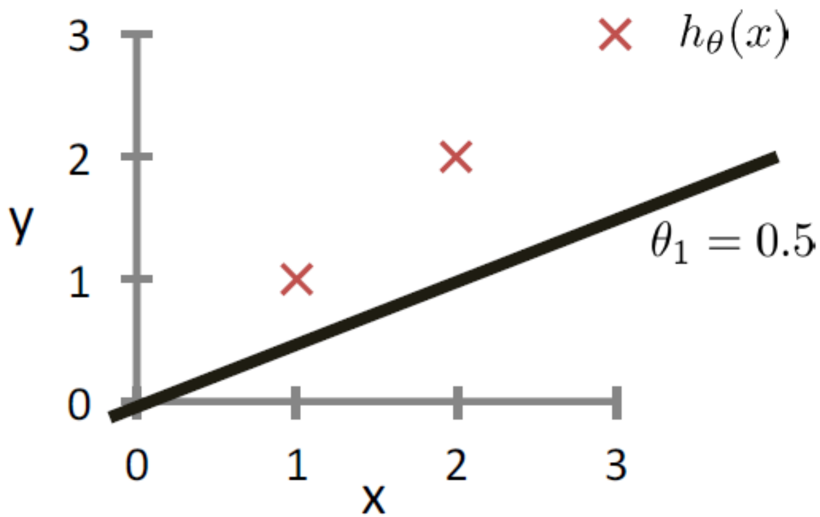

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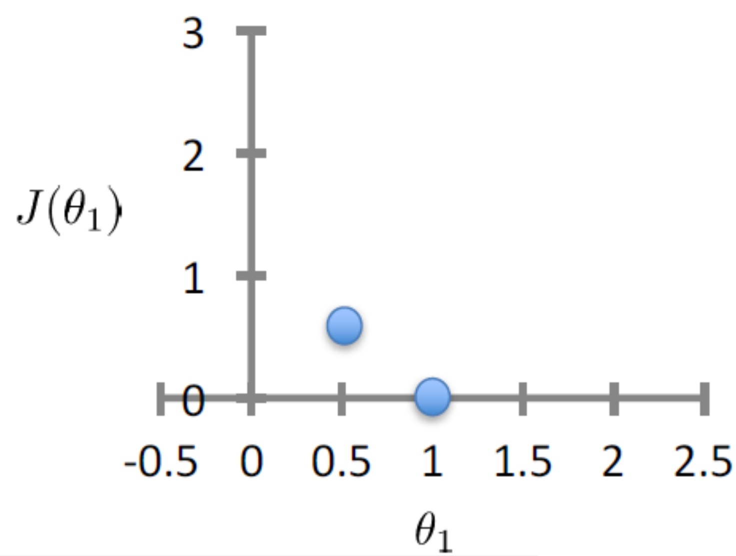


Based on example by Andrew Ng

$$J([0, 0.5]) = \frac{1}{2 \times 3}\left[(0.5-1)^2 + (1-2)^2 + (1.5-3)^2\right] \approx 0.58$$

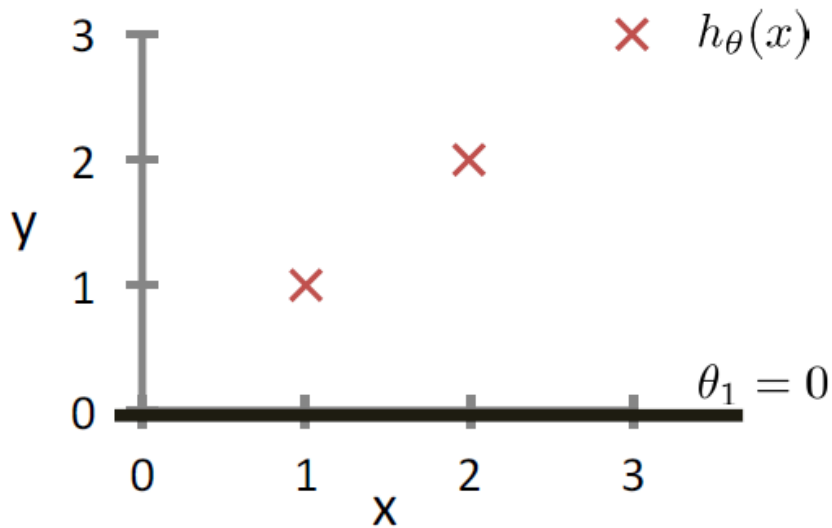
Intuition on MSE

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N}[h_\theta(x_i) - y_i]^2$$

For insight on J(), let's assume $x \in \mathbb{R}$ so $\boldsymbol{\theta} = [\theta_0, \theta_1]$

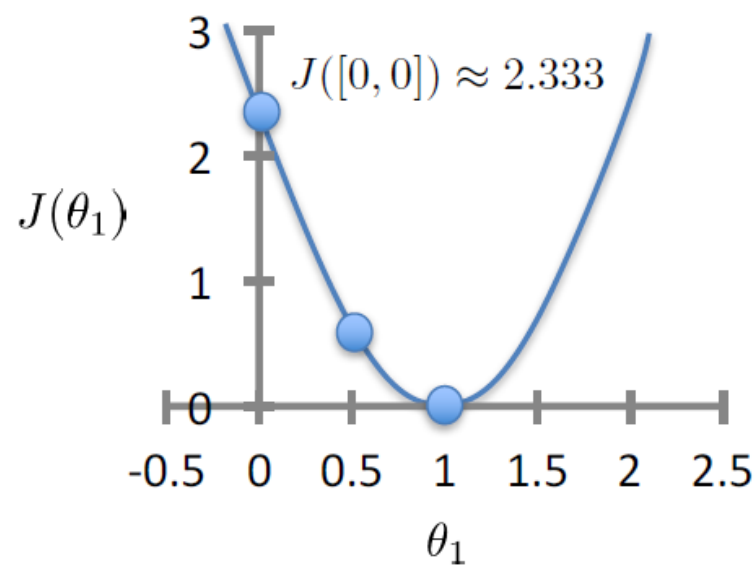
$h_\theta(x)$

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



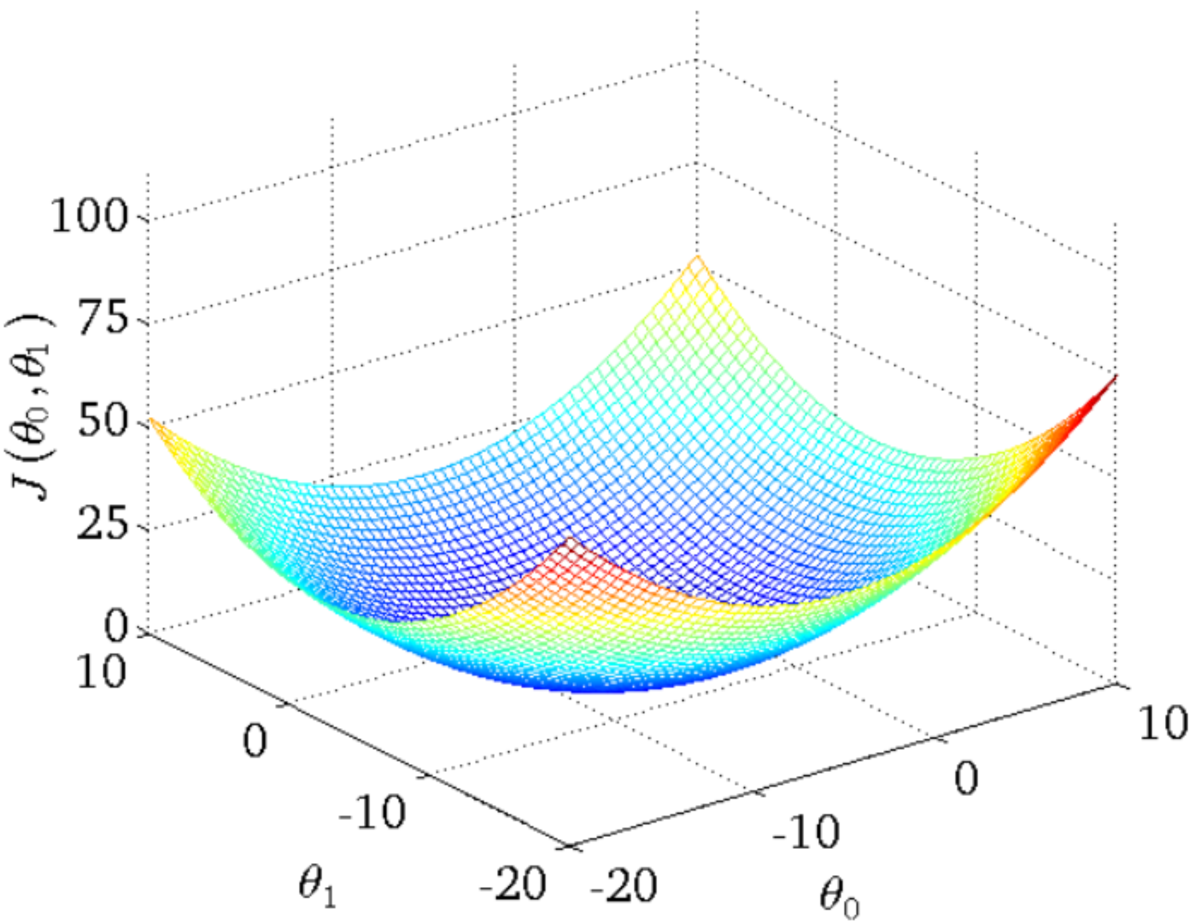
$J(\theta_1)$

(function of the parameter θ_1)



Based on example
by Andrew Ng

MSE function



Convex function, unique minimum

Solution for simple linear regression

- Dataset $x_i \in R, y_i \in R, h_\theta(x) = \theta_0 + \theta_1 x$
- $J(\theta) = \frac{1}{N}\sum_{i=1}^{N}(\theta_0 + \theta_1 x_i - y_i)^2$ MSE / Loss

$$\frac{\partial J(\theta)}{\partial \theta_0} = \frac{2}{N}\sum_{i=1N}(\theta_0 + \theta_1 x_i - y_i) = 0$$

$$\frac{\partial J(\theta)}{\partial \theta_1} = \frac{2}{N}\sum_{i=1}^{N} x_i(\theta_0 + \theta_1 x_i - y_i) = 0$$

- Solution of min loss

$$-\ \theta_0 = \bar{y} - \theta_1 \bar{x}$$

$$-\ \theta_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2}$$

$$\bar{x} = \frac{\sum_{i=1}^{N} x_i}{N}$$

$$\bar{y} = \frac{\sum_{i=1}^{N} y_i}{N}$$

Relationship between Two Random Variables

- Model X (feature / predictor) and Y (response) as two random variables
- Fit of simple linear regression depends on dependence between X and Y
- Covariance
  - Measures the strength of relationship between two random variables
- Pearson correlation
  - Normalized between [-1,1]
  - Proportional to covariance

Covariance

- X and Y are random variables
- $Cov(X,Y) = E\left[\left(X - E(X)\right)\left(Y - E(Y)\right)\right]$
- Properties

$$
\begin{aligned}
&\text{(i)} \quad \mathrm{Cov}(X,Y) = \mathrm{Cov}(Y,X) \\
&\text{(ii)} \quad \mathrm{Cov}(X,X) = \mathrm{Var(X)} \\
&\text{(iii)} \quad \mathrm{Cov}(aX,Y) = a\,\mathrm{Cov}(X,Y) \\
&\text{(iv)} \quad \mathrm{Cov}\left(\sum_{i=1}^{n} X_i, \sum_{j=1}^{m} Y_j\right) = \sum_{i=1}^{n}\sum_{j=1}^{m} \mathrm{Cov}(X_i, Y_j)
\end{aligned}
$$

Covariance

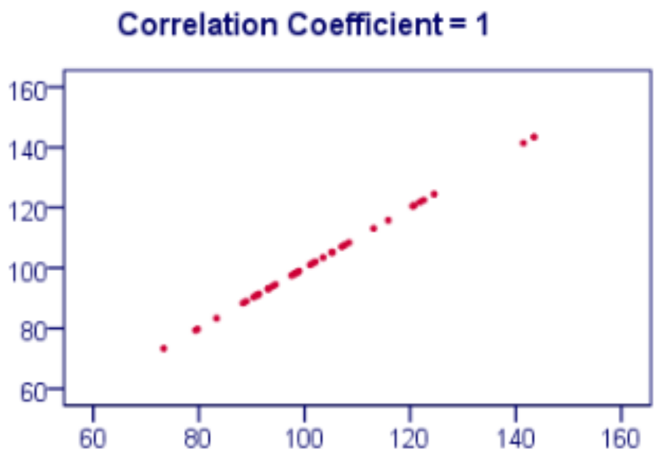
- X and Y are random variables
- Definition:
  - $Cov(X,Y) = E\left[\left(X - E(X)\right)\left(Y - E(Y)\right)\right]$
- Can derive that:
  - $Cov(X,Y) = E[XY] - E[X]E[Y]$
- If X and Y are independent then:
  - $E[XY] = E[X]E[Y]$
  - $Cov(X,Y) = 0$

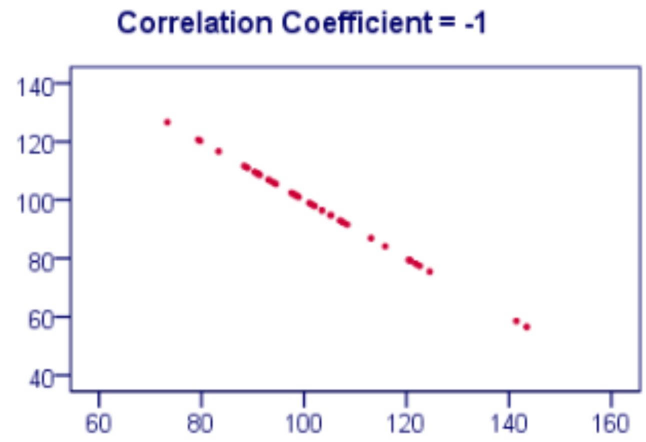
Pearson Correlation

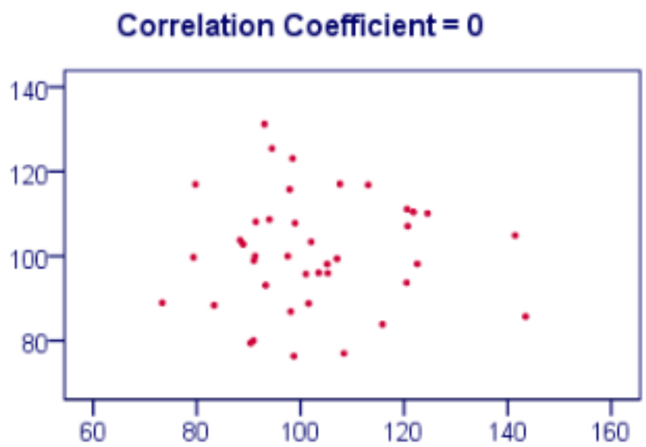
$$\rho = \mathrm{Corr}(X,Y) = \frac{\mathrm{Cov(X,Y)}}{\sigma_X \sigma_Y} \in [-1,1]$$

Standard deviation

$$\sigma_X = \sqrt{Var(X)}$$

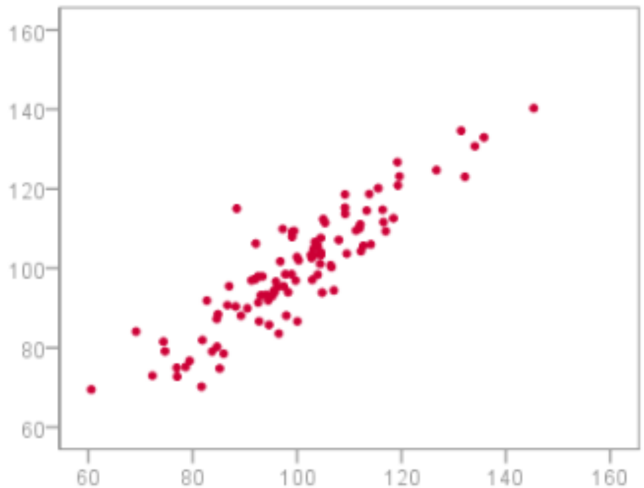




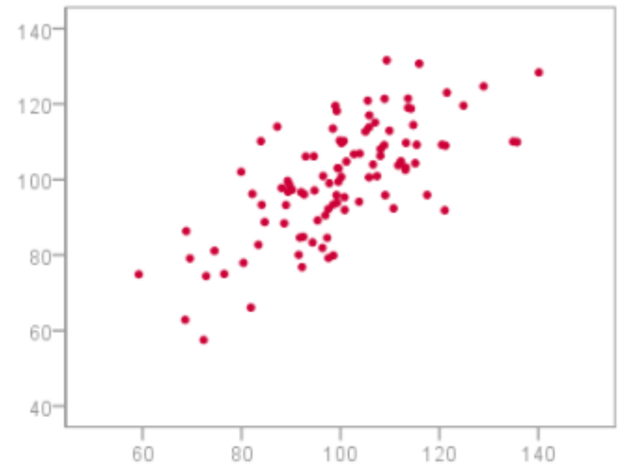


Positive/Negative Correlation

Positive Correlation

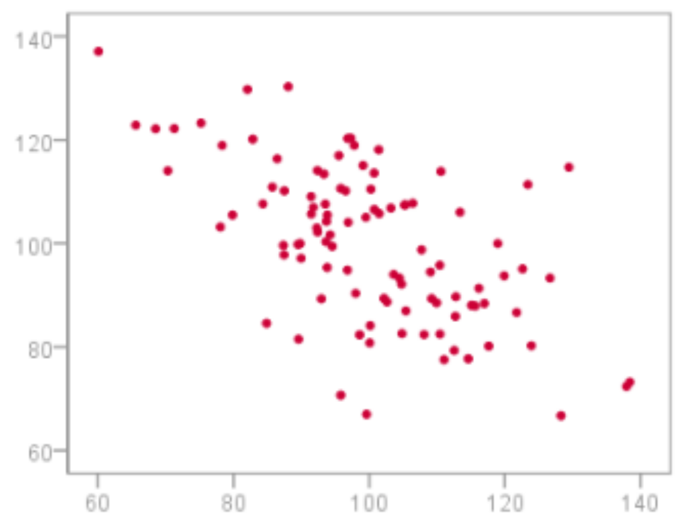


r = 0.9



r = 0.7

Negative Correlation



r = -0.6

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How Well Does the Model Fit?

- Correlation between feature and response
  - Pearson's correlation coefficient

$$\rho = \ Corr(X, Y) = \frac{\sum_{i=1}^{N}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{N}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{N}(y_i - \bar{y})^2}} = \frac{\mathrm{Cov}(\mathrm{X}, \mathrm{Y})}{\sigma_X \sigma_Y}$$

- Measures linear dependence between X and Y
- Positive coefficient implies positive correlation
  - The closer to 1 the coefficient is, the stronger the correlation
- Negative coefficient implies negative correlation
  - The closer to -1 the coefficient is, the stronger the correlation
- $\theta_1 = \frac{\sum \ (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} = \frac{\mathrm{Cov}(\mathrm{X,Y})}{Var[X]}$
- If σ_X = σ_Y, then $\theta_1 = \mathrm{Corr}(\mathrm{X}, \mathrm{Y})$

Regression vs Correlation

- Correlation
  - Find a numerical value expressing the relationship between variables
- Regression
  - Estimate values of response variable on the basis of the values of predictor variable
- The slope of linear regression is related to correlation coefficient
- Regression scales to more than 2 variables, but correlation does not