CS60050
Machine Learning

Linear Regression Part 1

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Dataset of living area and price of houses in a city

Living area (feet^2)	Price (1000\$s)
2104	400
1600	330
2400	369
1416	232
3000	540
⋮	⋮

← Training Set

Predict → $\boxed{5000}$ → $\boxed{?}$

m = number of **training examples**

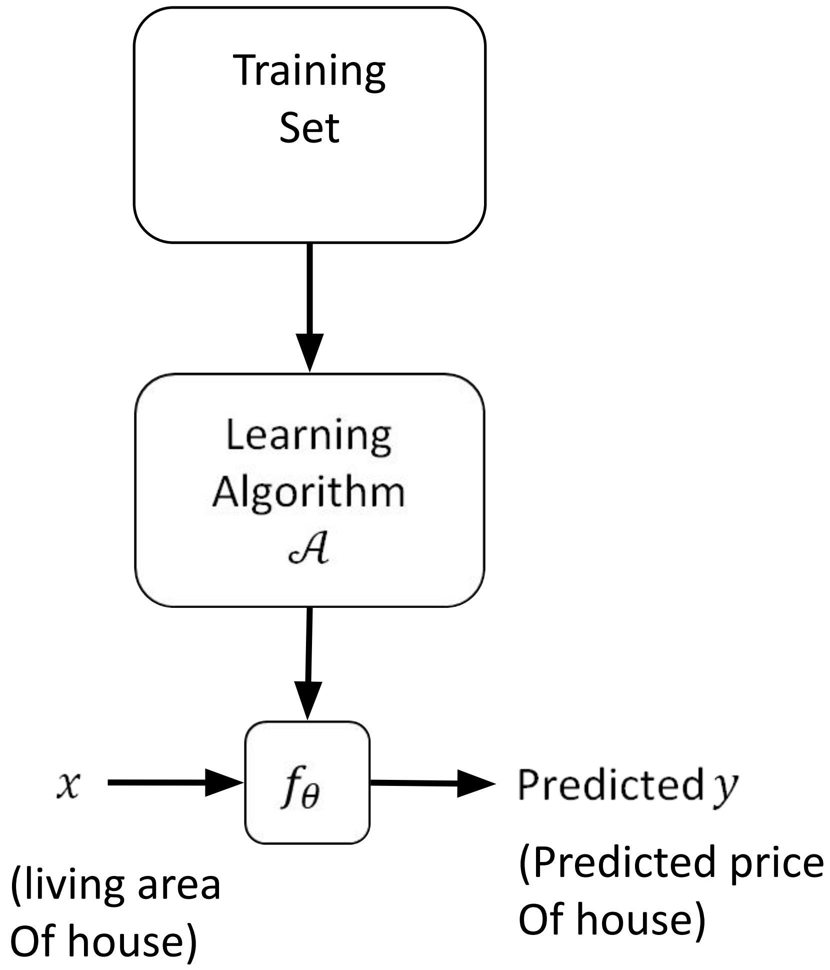
x_i = input variables / features

y_i = output variables / "target" variables

(x_i, y_i) - i^{th} training example of the training set

Regression

How to use the training set?



- Learn a function $f(x)$, so that $f(x)$ is a good predictor for the corresponding value of y
- f: hypothesis function

How to represent hypothesis? (linear?)

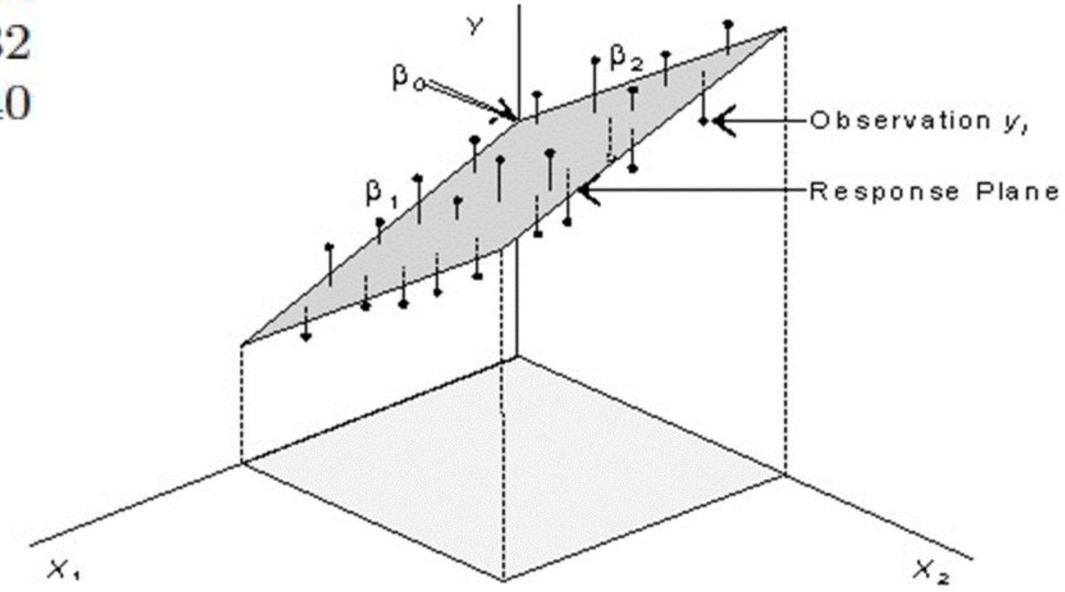
- $$\hat{y} = f_\theta(x) = \theta_0 + \theta_1 x$$

- θ_i are **parameters**
- $\boldsymbol{\theta}$: vector of all the parameters

- We assume
  - y is a linear function of x
- How to learn the values of the parameters θ_i ?

Multivariate Regression

Living area (feet^2)	#bedrooms	Price (1000\$s)
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540
⋮	⋮	⋮

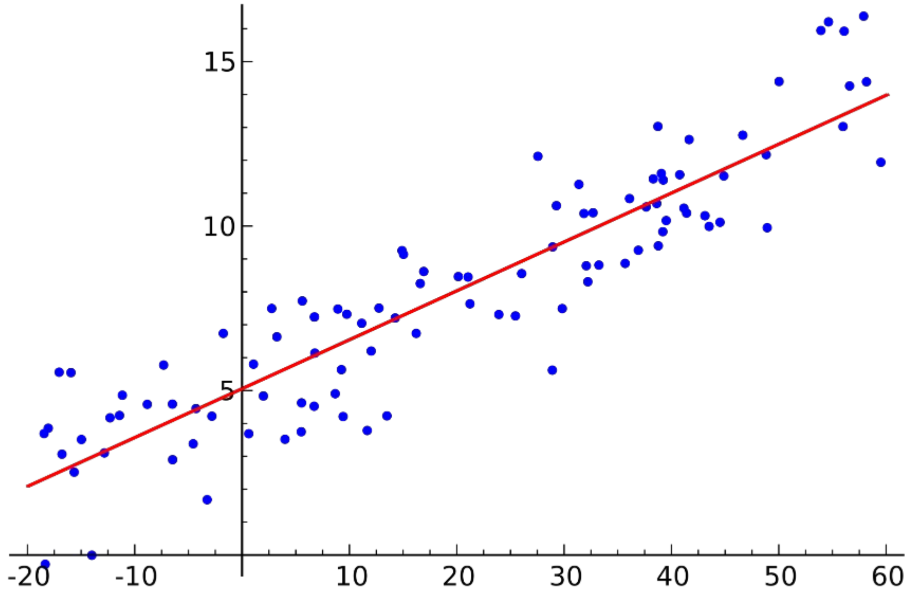


- n features
- m training examples
- $\left(x^{(i)}, y^{(i)}\right)$: ith training example

- $y = f_\theta(\mathrm{x}) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$

Intuition of hypothesis function

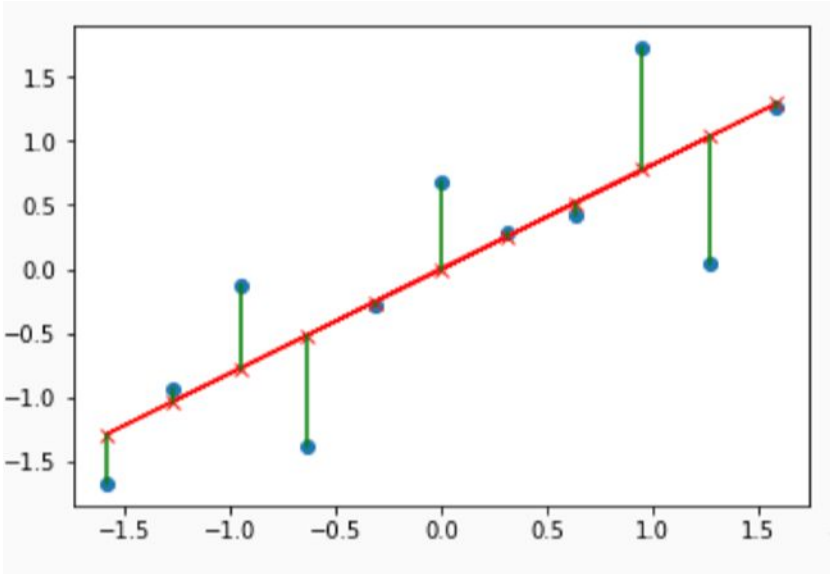
- $f_\theta(\mathrm{x}) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$



Two equivalent questions:

1. Which is the best straight line to fit the data?
2. How to learn the values of the parameters θ_i ?

Cost function



$$e^{(i)} = \widehat{y^{(i)}} - y^{(i)} = f_\theta\left(x^{(i)}\right) - y^{(i)}$$

prediction error for ith training example

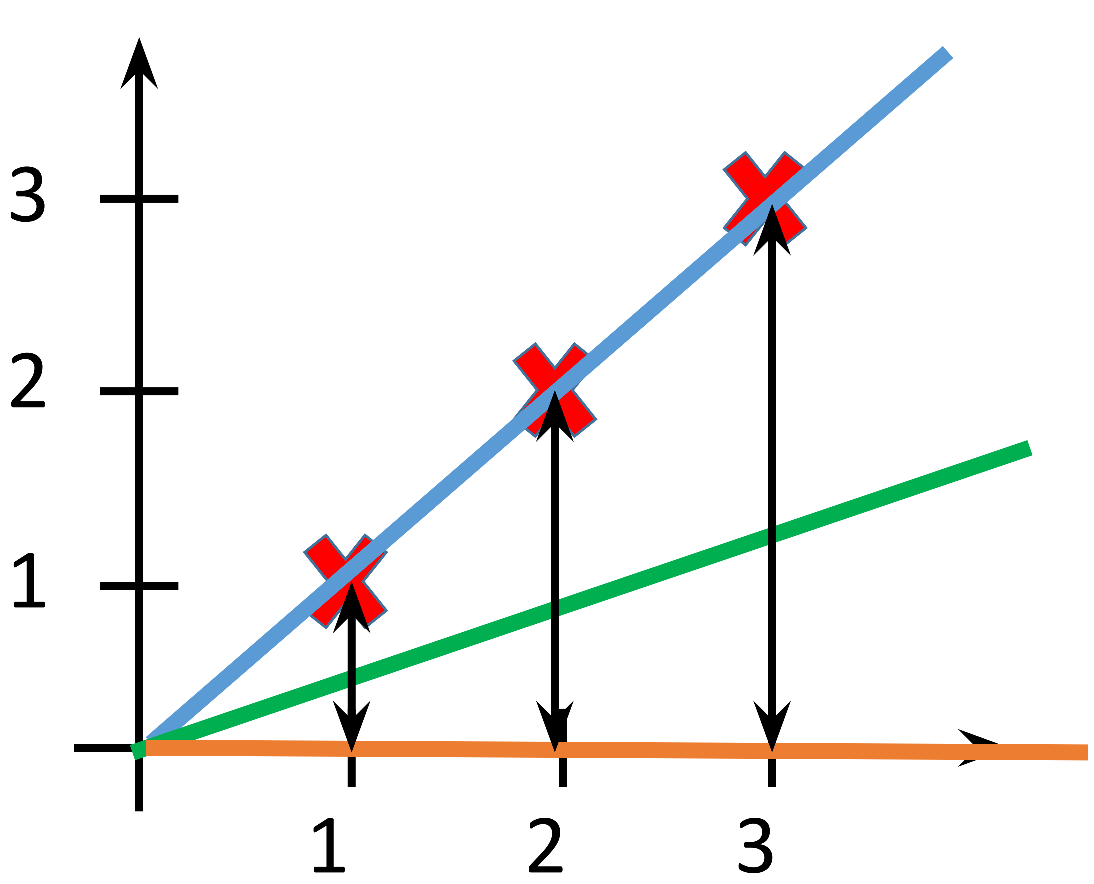
- $$loss(\bar{\theta}) = \frac{1}{2m}\sum_{i=1}^{m}\left(f_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2$$

Choose parameters $\bar{\theta}$ so that

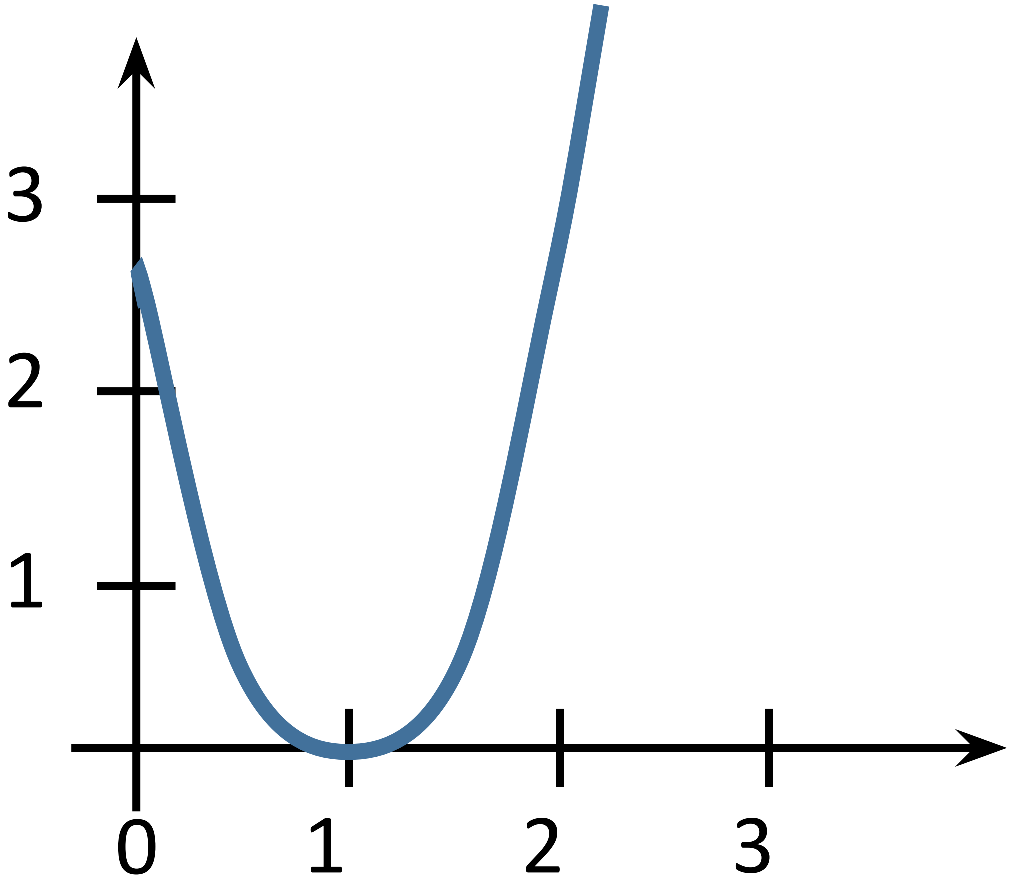
$loss(\bar{\theta})$ is minimized

$$\underset{\bar{\theta}}{\text{minimize}}\, J(\bar{\theta})$$

$f_\theta(x)$: function of x for fixed θ

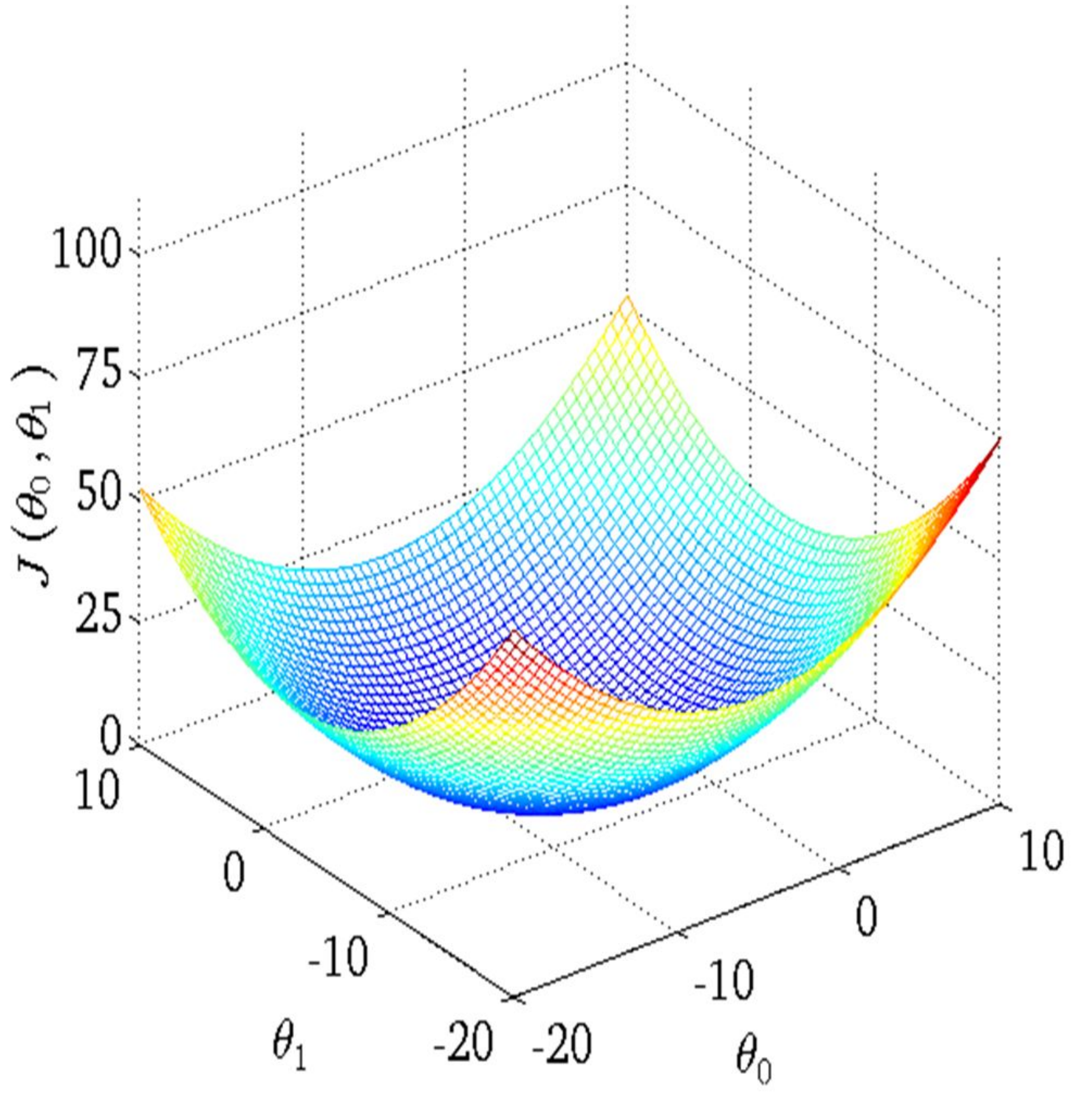


$loss(\theta)$, function of θ_0, θ_1



Cost Function

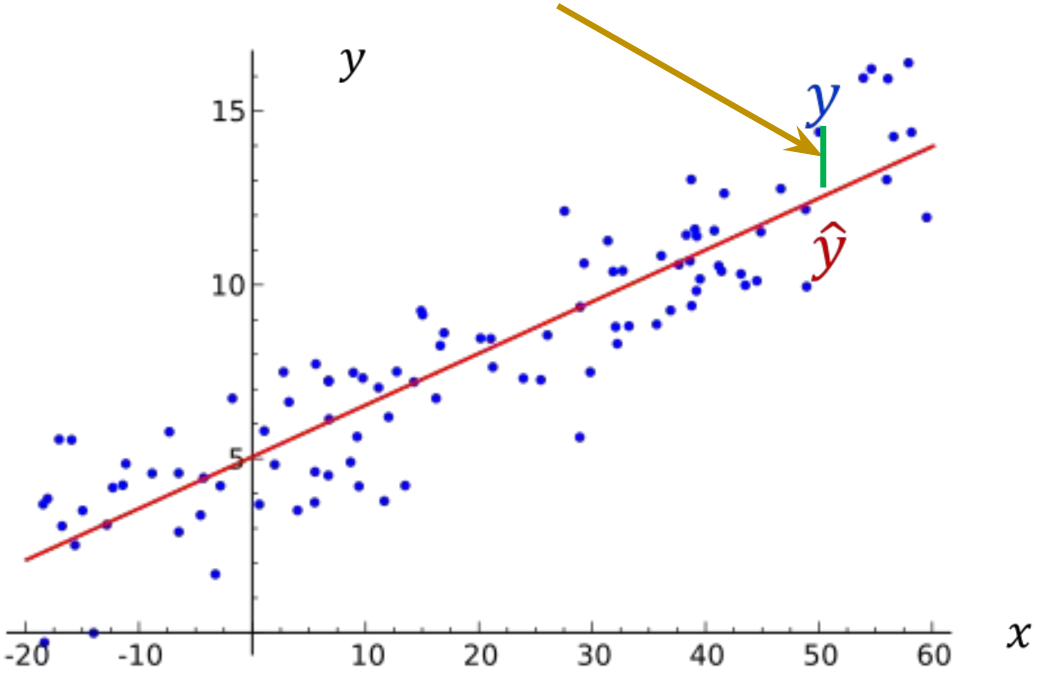
When loss is a function of both θ_0 and θ_1



Linear Regression

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

The loss is the squared loss $L_2(\hat{y}, y) \; = \; (\hat{y} - y)^2$



Data (x, y) pairs are the blue points.
The model is the red line.

Optimization objective: Find model parameters θ that will minimize the loss.

Linear Regression

- The total loss across all points is

$$L = \sum_{i=1}^{m} \left(\widehat{y^{(i)}} - y^{(i)}\right)^2$$

$$= \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)}\right)^2$$

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

We want the optimum values of θ_0, θ_1 that will minimize the sum of squared errors. Two approaches:

1. Analytical solution via mean squared error
2. Iterative solution via MLE and gradient ascent

Learning as Optimization Problem

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

Parameters:

θ_0, θ_1

Cost Function:

$$\ell oss(\theta) = \sum_{i=1}^{m} \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

$$= \sum_{n=1}^{m} \left(y_n - f_\theta\left(x^{(i)}\right)\right)^2$$

Goal:

$$\min_{\theta_0, \theta_1} loss(\theta_0, \theta_1$$

Linear Regression: Analytic Solution

- Since the loss is differentiable, we set

$$\frac{dL}{d\theta_0} = 0 \quad \text{and} \quad \frac{dL}{d\theta_1} = 0$$

$$L = \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)}\right)^2$$

We want the loss-minimizing values of $\boldsymbol{\theta}$, so we set

$$\frac{dL}{d\theta_1} = 0 = 2\theta_1 \sum_{i=1}^{m} \left(x^{(i)}\right)^2 + 2\theta_0 \sum_{i=1}^{m} x^{(i)}$$

$$\frac{dL}{d\theta_0} = 0 = 2\theta_1 \sum_{i=1}^{m} x^{(i)} + 2\theta_0 m - 2 \sum_{i=1}^{m} y^{(i)}$$

These being linear equations of θ, have a unique closed form solution

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

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

Multivariate Linear Regression

- $x \in \mathcal{R}^d$

$$\hat{y} = f(x;\ \theta) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ \dots + \theta_d x_d$$

Define $x_0 = 1$ $\quad f(x;\ \theta) = \theta^T \mathbf{x}$

$$\begin{bmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \vdots \\ \hat{y}^{(m)} \end{bmatrix} = \begin{bmatrix} {x_0}^{(1)} & {x_1}^{(1)} & {x_2}^{(1)} & \cdots & {x_d}^{(1)} \\ {x_0}^{(2)} & {x_1}^{(2)} & {x_2}^{(2)} & \cdots & {x_d}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ {x_0}^{(m)} & {x_1}^{(m)} & {x_2}^{(m)} & \cdots & {x_d}^{(m)} \end{bmatrix} \qquad \hat{y} = \mathbf{X\theta}$$

Cost Function:

$$loss(\boldsymbol{\theta}) = loss(\theta_0, \theta_1, \dots, \theta_d) = \frac{1}{m}\left(\boldsymbol{\theta}^T \mathrm{x}^{(i)} - y^{(i)}\right)^2$$

Multivariate Linear Regression

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$$loss(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i}\left(\boldsymbol{\theta}^T \mathrm{x}^{(i)} - y^{(i)}\right)^2$$

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

$$J(\boldsymbol{\theta}) = \frac{1}{m}\left((\mathbf{X\theta})^T - \mathbf{y}^T\right)(\mathbf{X\theta} - \mathbf{y})$$

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

$$loss(\boldsymbol{\theta}) = \frac{1}{m}\{\theta^T(X^TX)\theta - \theta^T X^T y - y^T X\,\theta + y^T Y\}$$

$$= \frac{1}{m}\{\theta^T(X^TX)\theta - (X^Ty)^T\theta - (X^Ty)^T\,\theta + y^T Y\}$$

$$= \frac{1}{m}\{\theta^T(X^TX)\theta - 2(X^Ty)^T\theta + y^T Y\}$$

Multivariate Linear Regression

- Equating the gradient of the cost function to 0,

$$\nabla_\theta loss(\,\boldsymbol{\theta}\,) = \frac{1}{m}\{2\mathbf{X}^T\mathbf{X}\boldsymbol{\theta} - 2\mathbf{X}^T\mathbf{y} + 0\} = 0$$

$$\mathbf{X}^T\mathbf{X}\boldsymbol{\theta} - \mathbf{X}^T\mathbf{y} = 0$$

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

This gives a closed form solution, but another option is to use iterative solution

$$\frac{\partial loss(\theta)}{\partial \theta_j} = \frac{1}{m}\sum_{i=1}^{m}\left(f_\theta\left(x^{(i)}\right) - y^{(i)}\right) x_j{}^{(i)}$$

Partial derivatives

- Let $y = f(\mathbf{x}) = f(x_1, x_2, \dots, x_n)$ be a multivariate function with *n* variables
  - The mapping is $f: \mathbb{R}^n \to \mathbb{R}$
- The ***partial derivative*** of *y* with respect to its *i*th parameter x_i is

$$\frac{\partial y}{\partial x_i} = \lim_{h \to 0} \frac{f(x_1, x_2, \dots, x_i + h, \dots, x_n) - f(x_1, x_2, \dots, x_i, \dots, x_n)}{h}$$

- To calculate $\frac{\partial y}{\partial x_i}$, we can treat $x_1, x_2, \dots, x_{i-1}, \quad x_{i+1} \dots, x_n$ as constants and calculate the derivative of *y* only with respect to x_i
- For notation of partial derivatives, the following are equivalent:

$$\frac{\partial y}{\partial x_i} = \frac{\partial f}{\partial x_i} = \frac{\partial}{\partial x_i} f(\mathbf{x}) = f_{x_i} = f_i = D_i f = D_{x_i} f$$

Multidimensional derivative: Gradient

- ***Gradient*** vector: The gradient of the multivariate function $f(\mathbf{x})$ with respect to the *n*-dimensional input vector $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T$, is a vector of *n* partial derivatives

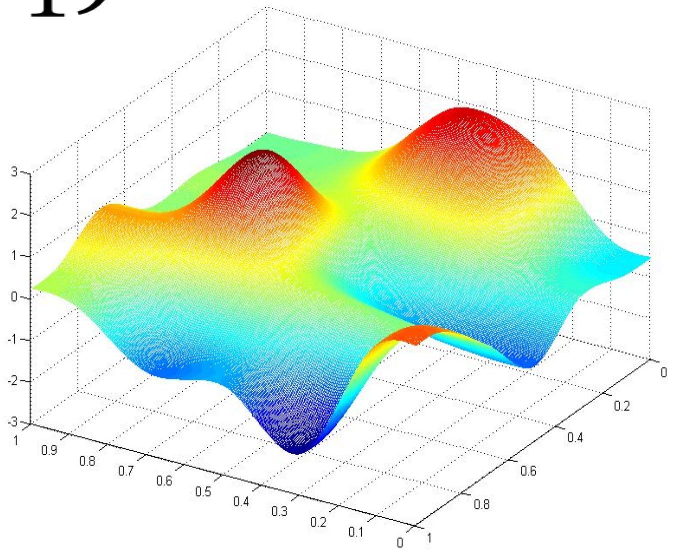
$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \left[\frac{\partial f(\mathbf{x})}{\partial x_1}, \frac{\partial f(\mathbf{x})}{\partial x_2}, \ldots, \frac{\partial f(\mathbf{x})}{\partial x_n}\right]^T$$

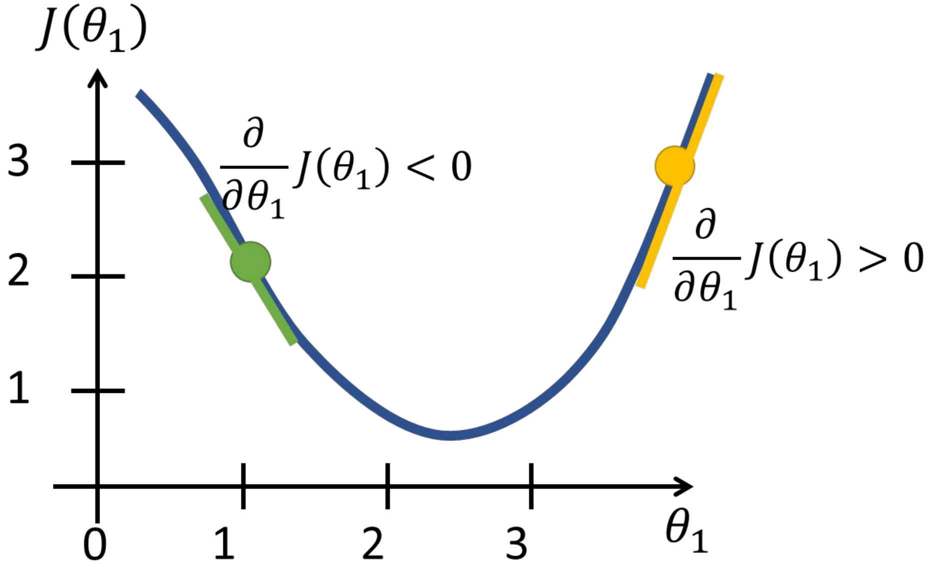
- In ML, the gradient descent algorithm relies on the opposite direction of the gradient of the loss function $\mathcal{L}$ with respect to the model parameters θ ($\nabla_\theta \mathcal{L}$) for minimizing the loss function

Minimizing cost function & Gradient Descent

Minimizing function $loss(\theta_0, \theta_1)$

- Start with some θ_0, θ_1
- Keep changing θ_0, θ_1 to reduce $loss(\theta_0, \theta_1)$
- until we end up at a minimum

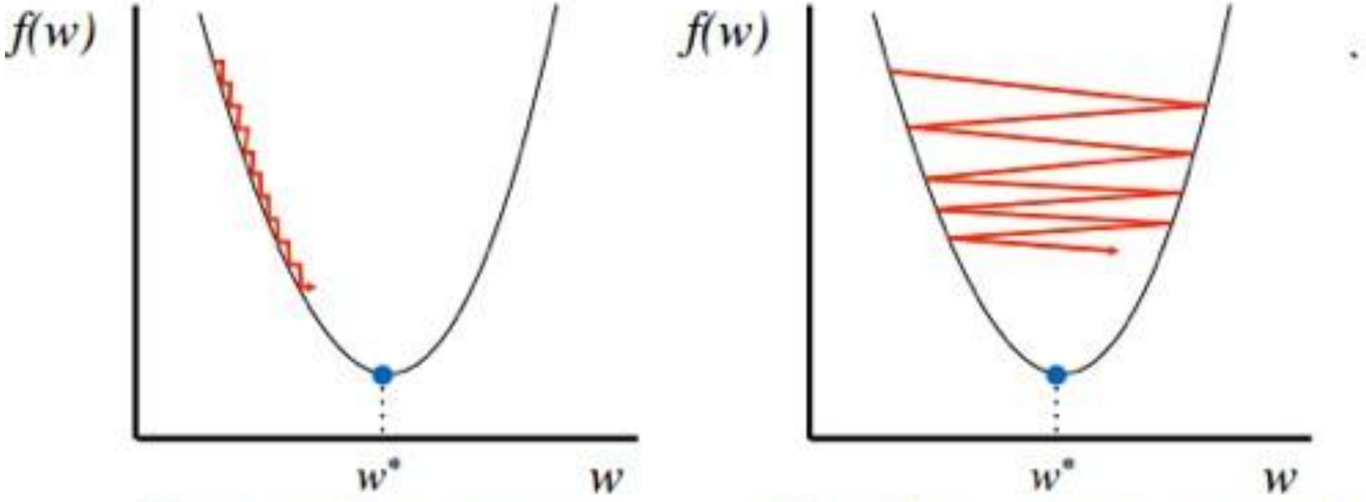




$$\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial\theta_1} loss(\theta_1)$$

Step Size α

- α Determines how quickly training loss goes down; hence "learning rate"



Too small: converge very slowly

Too big: overshoot and even diverge

Computing partial derivatives

$$loss(\bar{\theta}) = \frac{1}{2m}\sum_{i=1}^{m}\left(f_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2$$

$$\frac{\partial}{\partial\theta_j} loss(\bar{\theta}) = \frac{1}{m}\sum_{i=1}^{m}\left(f_\theta\left(x^{(i)}\right) - y^{(i)}\right) x_j^{(i)}$$

Repeat until convergence{

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

Equivalently

$$\theta_j := \theta_j - \alpha \frac{1}{m}\sum_{i=1}^{m}\left(f_\theta\left(x^{(i)}\right) - y^{(i)}\right) x_j^{(i)}$$

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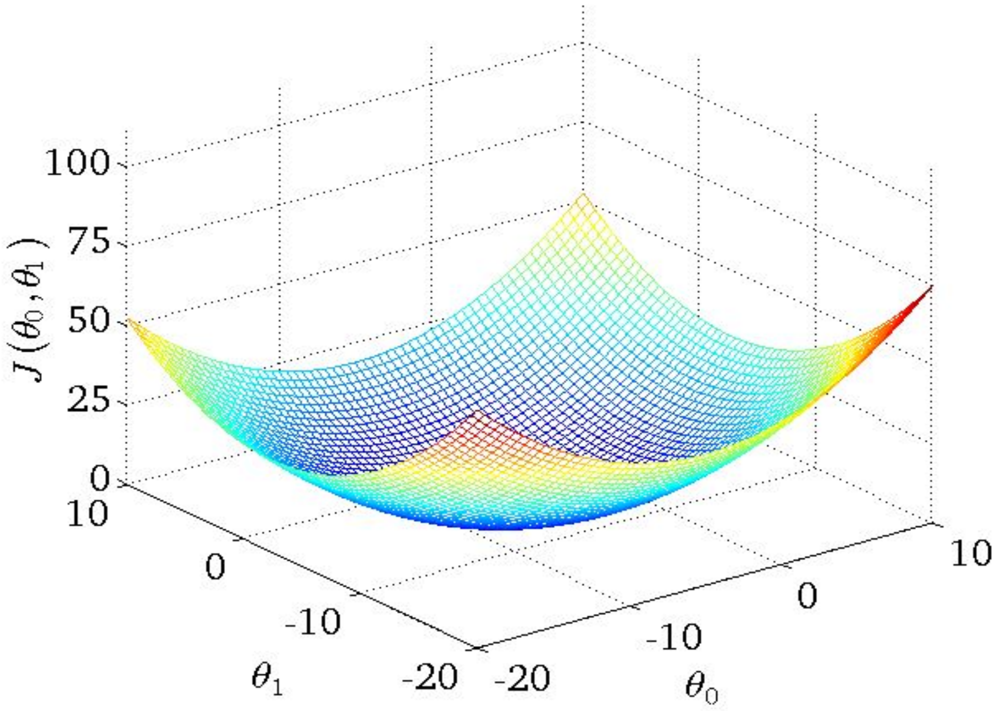
Convergence

- The cost function in linear regression is always a convex function – always has a single global minimum
- So, gradient descent will always converge



Batch gradient descent

- "Batch": Each step of gradient descent uses all the training examples

Repeat until convergence{

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{\boxed{m}} \left(f_\theta\left(x^{(i)}\right) - y^{(i)} \right)$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{\boxed{m}} \left(f_\theta\left(x^{(i)}\right) - y^{(i)} \right) x^{(i)}$$

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