Week 2: Single Variable Linear Regression

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Notations

Let a dataset $D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$ be a set of N pairs (x_i, y_i), where $x_i \in \mathbb{R}^d$ is a feature vector (independent variable) and $y_i \in \mathbb{R}$ (dependent variable).

Function approximation or hypothesis (model):

$$f : X \to Y, \quad f : \mathbb{R}^{nxd} \to \mathbb{R}^{nx1}$$

Model Representation

- For a single variable linear regression: $d = 1$
- Model: $h_\theta(x) = \theta_0 + \theta_1 x$
- θ: parameters, $\theta_j \in \mathbb{R}$, and $|\theta| = d + 1$
- Loss/Cost function (Mean Squared Error)

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

- Objective

$$\hat{\theta}_0, \hat{\theta}_1 = \arg\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$$

Example

x	y
0	1
2	1
3	4

Two possible hypotheses:

$h_\theta(x) = 3$, and MSE $= 3$

$h_\theta(x) = 1 + x$, and MSE $= 1.33$

Solution approach

1. **Analytical approach**: Normal equation

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

2. **Iterative approach**: Gradient Descent

Normal Equation Issues (1/2)

- Problem 1: $(X^T X)$ non-invertible
  - Example: redundant features
- Solution:
  - SVD (Singular Value Decomposition)
  - Moore–Penrose Pseudo-inverse

Normal Equation Issues (2/2)

- Problem 2: Computational complexity $O(n^3)$ for large feature sets (Why?).
- Solution: Use iterative approach (Gradient Descent)

Iterative approach: (Batch) Gradient Descent

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

Objective function (Mean Squared Error):

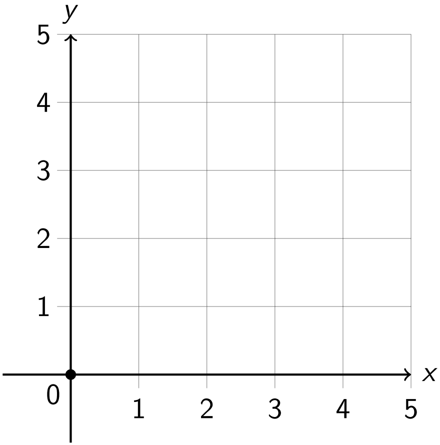
$$J(\theta_0, \theta_1) = \frac{1}{N} \sum_{i=1}^{N} (h_\theta(x_i) - y_i)^2$$

Goal:

$$\arg\min_{\theta_0, \theta_1} J(\theta_0, \theta_1)$$

Batch Gradient Descent (GD) is a way to minimize an objective function $J(\theta)$ by updating θ in the opposite direction of the gradient of J, i.e., $\nabla J(\theta)$.

How J changes with θ:



Relation between J and two θ

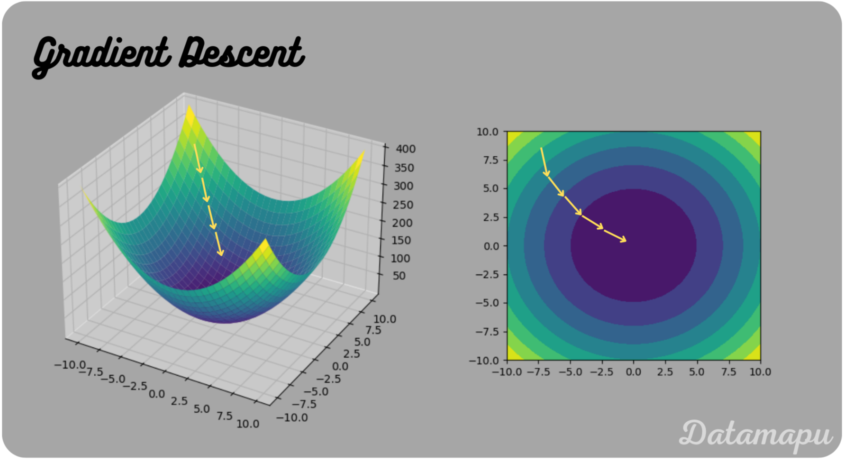


Figure: Relation between J and θ_0,θ_1

Batch GD equation

Loop until convergence:

$$\theta_j^{t+1} := \theta_j^t - \eta \frac{\partial}{\partial \theta_j^t} J(\theta_0^t, \theta_1^t), \text{where } j = 0, 1,$$

$$t = 0, 1, 2, ...$$

and η 'eta' is a learning rate

Take a look at $\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$. We get,

$$\theta_j^{t+1} := \theta_j^t - \eta \frac{1}{N} \sum_{i=1}^{N} \frac{\partial (h_\theta(x_i) - y_i)^2}{\partial \theta_j^t}, \quad j = 0, 1$$

Update equation of Batch GD (I)

Loop until convergence (stop):

$$\theta_j^{t+1} := \theta_j^t - \eta \frac{1}{N} \sum_{i=1}^{N} (h_\theta(x_i) - y_i) x_i, \quad j = 0, 1$$

$$\theta_0^{t+1} := \theta_0^t - \eta \frac{1}{N} \sum_{i=1}^{N} (h_\theta(x_i) - y_i) x_{i,0}$$

$$\theta_1^{t+1} := \theta_1^t - \eta \frac{1}{N} \sum_{i=1}^{N} (h_\theta(x_i) - y_i) x_{i,1}$$

Stopping criteria:

- Max iterations or
- $|MSE_{t+1} - MSE_t| < epsilon$

Update equation of Batch GD (II)

Limitations:

- Need to define η
- Slow for large datasets (Big N)

Iterative VS Analytical approach

Iterative	**Analytical**
Need η	No need η
Workable for large d	Not workable for large d
Need feature scaling	No feature scaling
No invertibility issue	Invertibility issue
$O(n^2)$	$O(n^3)$

Exercise 1: Solve Both Approaches

x	y
2	12
5	9
1	6

1. Analytical: $\theta = (X^T X)^{-1} X^T y$
2. Iterative: Batch GD, define $\theta_0, \theta_1 = 0.1$, $\eta = 0.01$, $\#\text{iter} = 3$.

Reference

- Marill,K.A. (2004). Advanced statistics: linear regression, partI: simple linear regression. Academic emergency medicine, 11(1), 87-93.