- Different types of machine learning
- Linear models
- Terminology in linear model problems
- 1-dimensional OLS and minimizing the loss function
- Interpreting parameters in an OLS equation
- Limitations of using OLS through Anscombe's Quartet
- Multivariate OLS models and an example problem
- Using matrix foundation to solve the OLS problem
- The pros and cons of using OLS regression

Learning Objectives

- Understand ordinary least squares (OLS)

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Types of Machine Learning

- Unsupervised Learning
  - Finding structure in data
- Supervised Learning
  - Predict from given data

Introduction

- Objective
  - What is a linear model?
  - Why use linear models?

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Example of Use

- Example of Use
- Building Blocks of Later Techniques

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Terminology

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- Definitions
  - Features (covariates or predictors)
  - Labels (variates or targets)
  - Regression
  - Classification

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Definition of 1-Dimension OLS

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- The Problem Statement
- The Loss Function

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Solution of OLS

- Derivation
- Optimal Choices

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Interpretation

- Interpretation of a
- Interpretation of L

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Anscombe's Quartet

- Anscombe's Quartet

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Multivariable OLS

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- Definition of Model
  - Data matrix
  - The loss function

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Optimization

- A Few Facts from Matrix Calculus
- Minimizing the Loss

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OLS Pros and Cons

- OLS
  - Pros
  - Cons

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Types of Machine Learning

To get us started, the video below explains classifying training data so that humans can ide

the data structures, or make predictions from the data.

Two types of machine learning covered in this video include:

Unsupervised Learning

Supervised Learning

Topics

- Unsupervised Learning
  - Finding structure in data
- Supervised Learning
  - Predict from given data

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Unsupervised Learning

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Finding structure in data

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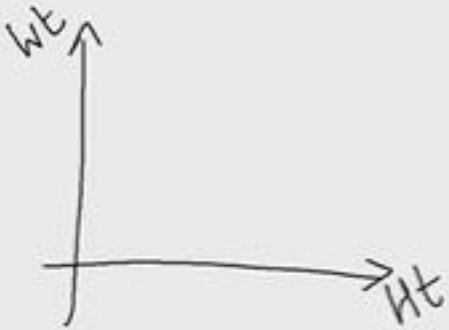
Supervised Learning

Predict from given data



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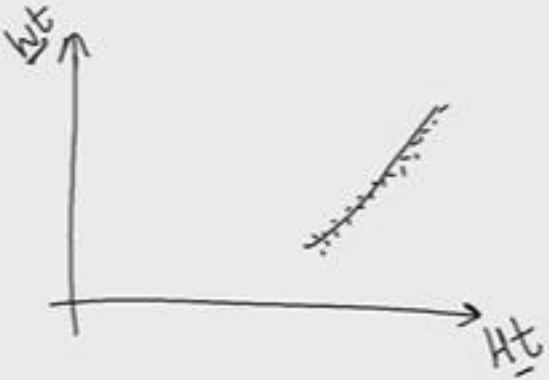
Supervised Learning

Predict from given data

Classification



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Supervised Learning

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Ordinary least squares (OLS) and **logistic regression** are methods of these two types of supervised learning problem.

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Supervised Learning

aws training and certification

Ordinary least squares (OLS) and **logistic regression** are methods of these two types of supervised learning problem.

OLS - Regress

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Supervised Learning

aws training and certification

Ordinary least squares (OLS) and **logistic regression** are methods of these two types of supervised learning problem.

OLS - Regression

Log. Reg - Clo

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Supervised Learning

aws training and certification

Ordinary least squares (OLS) and **logistic regression** are methods of these two types of supervised learning problem.

OLS - Regression

Log. Reg - Classification

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Supervised Learning

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Ordinary least squares (OLS) and **logistic regression** are methods of these two types of supervised learning problem.

OLS - Regression

Log. Reg - Classification

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Introduction to Linear Models

This video explains how linear models look and what they are used for. Take a moment to explore linear models before you begin.

What is a linear model?

In linear modeling, the relationship between each individual input variables and the output is a straight line. Slopes of such lines become the coefficients of the linear equation.

An example of linear notation

$$y_i = a_0 + a_1x_1 + a_2x_2 + \ldots$$

An example of linear notation

$$y_i = a_0 + a_1x_1 + a_2x_2 + \ldots$$

Why use linear models?

- Interpretable
- Low complexity
- Scalable

What is a Linear Model?

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$$\text{Housing price} = k_1(\text{Area}) + k_2(\#\text{bedrooms}) + k_3(\#\text{bathrooms})$$

Housing prices

- Area
- #bedrooms
- #bathrooms

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What is a Linear Model?

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$$\text{Housing price} = k_1(\text{Area}) + k_2(\#\text{bedrooms}) + k_3(\#\text{bathrooms})$$

Housing prices

- Area
- #bedrooms
- #bathrooms

$$y_i = a_0 + a_1 x_1 + a_2 x_2 + \cdots$$

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Why Use Linear Models?

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- Interpretable
- Low complexity
- Scalable
- Baseline

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Example of Use

Machines encounter certain problems when trying to identify handwritten digits. Before watching the video below, take a moment to compare the performance of a regression model and a neural network model with regard to this challenge.

Handwriting Digit Recognition

MNIST Example

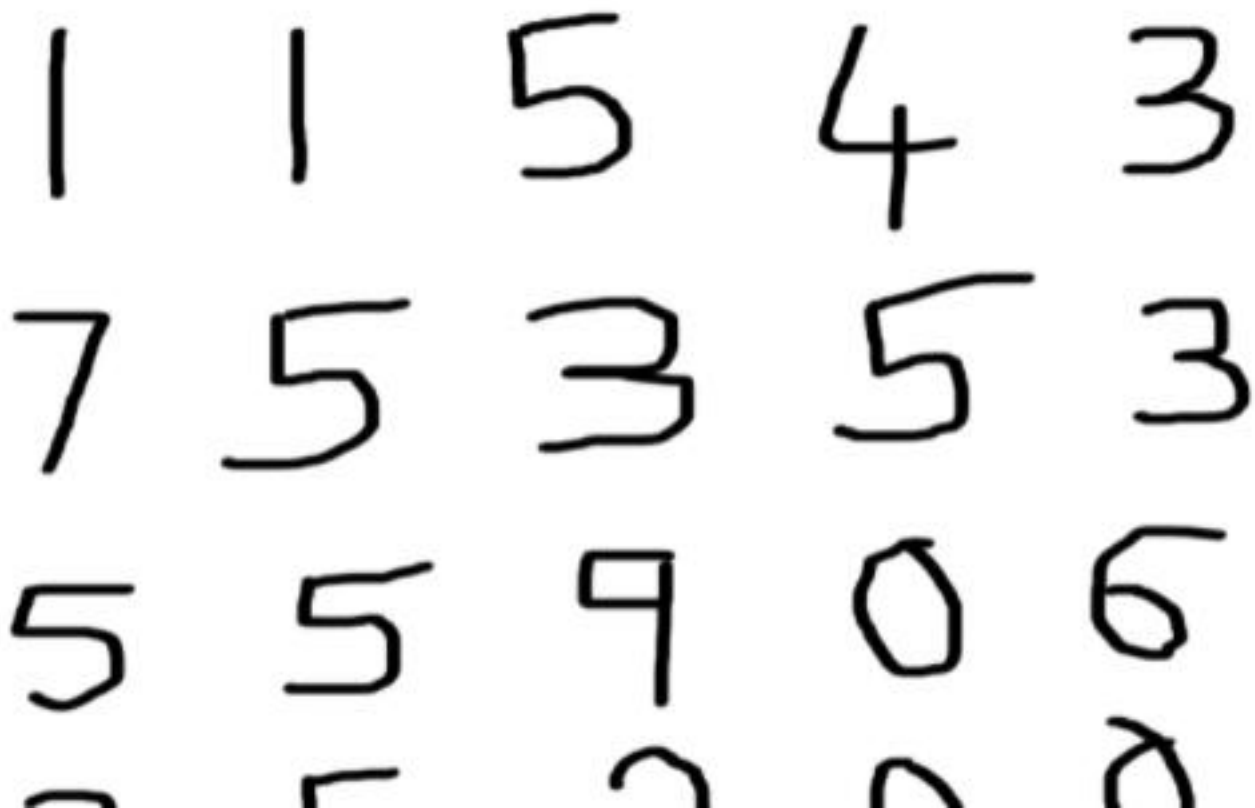
Handwriting Digit Recognition

MNIST Example

THE CHALLENGE | A NEURAL NETWORK SOLUTION | A LOGISTIC REGRESSION SOLUTION

The machine learning task is to identify what the digits are.

**data source: Modified National Institute of Standards and Technology(MNIST) database hand written digits.*



Handwriting Digit Recognition

MNIST Example

THE CHALLENGE	A NEURAL NETWORK SOLUTION	A LOGISTIC REGRESSION SOLUTION

Uses advanced regularization techniques via a neural network

- Is 99.79 % error free
- Takes about a day to train
- Requires significant expertise to achieve

Handwriting Digit Recognition

MNIST Example

THE CHALLENGE	A NEURAL NETWORK SOLUTION	A LOGISTIC REGRESSION SOLUTION

Uses logistic regression

- Is 92.5 % error free
- Takes seconds to train
- Can be done with (comparatively) less expertise

Example of Use

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MNIST is a common data set that contains images of handwritten digits. The machine learning task is to identify what the digits are.

*Data Source: Modified National Institute of Standards and Technology (MNIST) Database of Handwritten Digits

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Example of Use

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Logistic regression

- Is 92.5 percent error free
- Takes seconds to train
- Can be done with (comparatively) less expertise

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Building Blocks for Later Techniques

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More advanced techniques like neural networks are, mathematically, a little more complex than **stacking** logistic regression.

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Dataset References

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- Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. "Gradient-based learning applied to document recognition." Proceedings of the IEEE, 86(11):2278-2324, November 1998. Dataset available from http://yann.lecun.com/exdb/mnist/

The Problem Statement

$i = 1, \ldots, N$

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The Problem Statement

$i = 1, \ldots, N$, x = indepent var. y = dep. var.

$$y = ax + b$$

a, b constants.

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The Problem Statement

$i = 1, \ldots, N$, x = indepent var. y = dep. var.

$$y = ax + b$$

a, b constants

$$\hat{y}_i = ax_i + b$$

$$y_i = ax_i + b + \epsilon$$

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The Loss Function

$$\mathcal{L} = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

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Solutions a and b:

For an optimized model the loss function should be less.

Find the L minimum by equating the first derivatives of L to zero, and solving for the values of a and b for which L is minimum.

To best fit a collection matched input output pairs $\{x_i\}_{i=1}^{N}$ and $\{y_i\}_{i=1}^{N}$ with a function of the form $y = ax + b$ to minimize the mean squared error, you should pick:

$$a = \frac{\sum_i x_i y_i - \frac{1}{N}(\sum_i x_i)(\sum_i y_i)}{\sum_i x_i^2 - \frac{1}{N}(\sum_i x_i)^2} \qquad \left[= \frac{Cov(X,Y)}{Var(X)}\right]$$

$$b = \frac{1}{N}\sum_i y_i - \frac{a}{N}\sum_i x_i \qquad [= E[Y] - aE[X]]$$

These are exact solutions to the minimization problem.

Derivation

$$L = \sum_{i=1}^{N} (y_i - ax_i - b)^2$$

$$\underline{\min L}$$

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Derivation

$$L = \sum_{i=1}^{N} (y_i - ax_i - b)^2$$

$$\underline{\min L}$$

$$\frac{dL}{da} = 0 \quad , \quad \frac{dL}{db} = 0$$

$$\frac{dL}{da} = 0 \Rightarrow \sum_{i=1}^{N} 2(y_i - ax_i - b)($$

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Derivation

$$L = \sum_{i=1}^{N} (y_i - ax_i - b)^2$$

$$\underline{\min L}$$

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$$\frac{dL}{da} = 0 \Rightarrow \sum_{i=1}^{N} 2(y_i - ax_i - b)(+x_i) = 0$$

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Derivation

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$$L = \sum_{i=1}^{N} (y_i - ax_i - b)^2$$

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$$\frac{dL}{da} = 0 \Rightarrow \sum_{i=1}^{N} 2(y_i - ax_i - b)(+x_i) = 0$$

$$\sum_{i=1}^{N} x_i y_i - a \sum_{i=1}^{N} x_i^2 .$$

-4:16

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Derivation

$$\frac{dL}{db} = 0 \Rightarrow \sum_{i=1}^{N} +\cancel{2}(y_i - ax_i - b)(+1) = 0$$

$$\sum y_i - a\sum x_i - bN = 0$$

$$b = \frac{1}{N}\sum$$

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Derivation

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$$\frac{dL}{db} = 0 \Rightarrow \sum_{i=1}^{N} +\cancel{2}(y_i - ax_i - b)(+1) = 0$$

$$\sum y_i - a\sum x_i - bN = 0$$

$$\boxed{b = \frac{1}{N}\sum y_i - \frac{a}{N}\sum x_i} \quad -②$$

-2:37

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Derivation

$$\frac{dL}{db} = 0 \Rightarrow \sum_{i=1}^{N} +\cancel{2}(y_i - ax_i - b)(+1) = 0$$

$$\sum y_i - a\sum x_i - bN = 0$$

$$\boxed{b = \frac{1}{N}\sum y_i - \frac{a}{N}\sum x_i} \quad -②$$

From ①, ②

$$\sum_{i=1}^{N} x_i y_i - a\sum_{i=1}^{N} x_i^2 - b\sum x_i = 0$$

$$\Rightarrow \sum x_i y_i = a\sum x_i^2 + \sum x_i\left(\frac{1}{N}\sum y_i - \frac{a}{N}\sum x_i\right)$$

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Derivation

$$\frac{dL}{db} = 0 \Rightarrow \sum_{i=1}^{N} +\cancel{2}(y_i - ax_i - b)(+1) = 0$$

$$\sum y_i - a\sum x_i - bN = 0$$

$$\boxed{b = \frac{1}{N}\sum y_i - \frac{a}{N}\sum x_i} \quad — ②$$

From ①,

$$\sum_{i=1}^{N} x_i y_i - a\sum_{i=1}^{N} x_i^2 - b\sum x_i = 0$$

$$\Rightarrow \sum x_i y_i = a\sum x_i^2 + \sum x_i\left(\frac{1}{N}\sum y_i - \frac{a}{N}\sum x_i\right)$$

$$a = \frac{\sum x_i y_i - \frac{1}{N}\sum x_i \sum y_i}{\sum x_i^2 - \frac{1}{N}\left(\sum x_i\right)^2}$$

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Optimal Choices

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To best fit a collection matched input output pairs $\{x_i\}_{i=1}^N$ and $\{y_i\}_{i=1}^N$ with a function of the form $y = ax + b$ to minimize the mean squared error, you should pick:

$$a = \frac{\sum_i x_i y_i - \frac{1}{N}(\sum_i x_i)(\sum_i y_i)}{\sum_i x_i^2 - \frac{1}{N}(\sum_i x_i)^2} \qquad \left[= \frac{Cov(X,Y)}{Var(X)}\right]$$

$$b = \frac{1}{N}\sum_i y_i - \frac{a}{N}\sum_i x_i \qquad [= E[Y] - aE[X]]$$

These are **exact** solutions to the minimization problem.

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Optimal Choices

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These are **exact** solutions to the minimization problem.

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Interpretation

In the last video, you found the solutions for a and b. Now you will interpret a and b on a linear graph of x (input parameters) and y (output) to obtain a generalized condition for predicting y. You will also analyze the loss function with a and b values to understand a model's performance.

Interpretation of a and b

a – slope of the line (size of relationship between X and Y)
b – intercept

$$i.e.\ \ b = \begin{cases} \hat{y}, & x = 0 \\ 0, & x = \hat{x} \end{cases}$$

Interpretation of L

In general, $R^2 \in [0,1]$

Let's observe the model performance with the help of R^2 which is defined as. Keep in mind, L = loss function.

$$R^2 = 1 - \frac{Loss\ Function}{Var\ (y)} = 1 - \frac{MSE}{\bar{y}}$$

Interpretation of *a*, *b*

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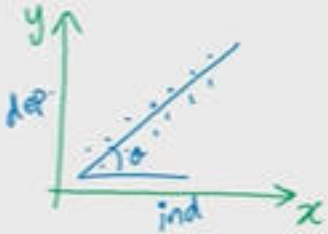
a = slope

→ effect



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Interpretation of *a*, *b*

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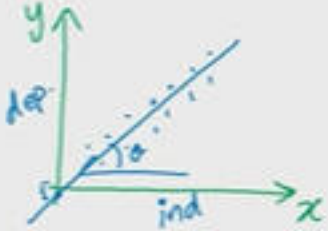
a = slope

→ effect size

b = intercept



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Interpretation of *a*, *b*

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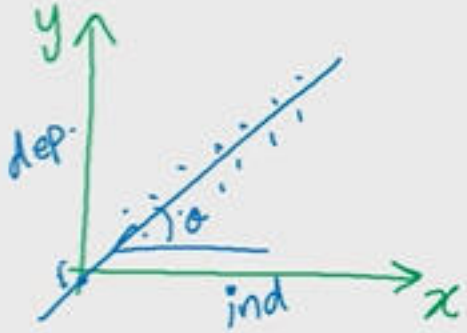
a = slope

→ effect size.

b = intercept

→ $\hat{y} = b$ when



-3:46

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Interpretation of L

$$L = \sum_{i=1}^{N} (y_i - \hat{y})^2$$

$$\hookrightarrow R^2$$

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Interpretation of L

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MSE, $L = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$

$\hookrightarrow R^2 = 1 - \frac{MSE}{Var(y)}$

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Interpretation of L

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MSE, $L = \sum_{i=1}^{N} (y_i - \hat{y})^2$

$\hookrightarrow R^2 = 1 - \frac{MSE}{Var(Y)}$ $(\hat{Y})$ $(\bar{Y})$

$R^2 \in [0, 1]$

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Topics

- Anscombe's Quartet

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Anscombe's Quartet

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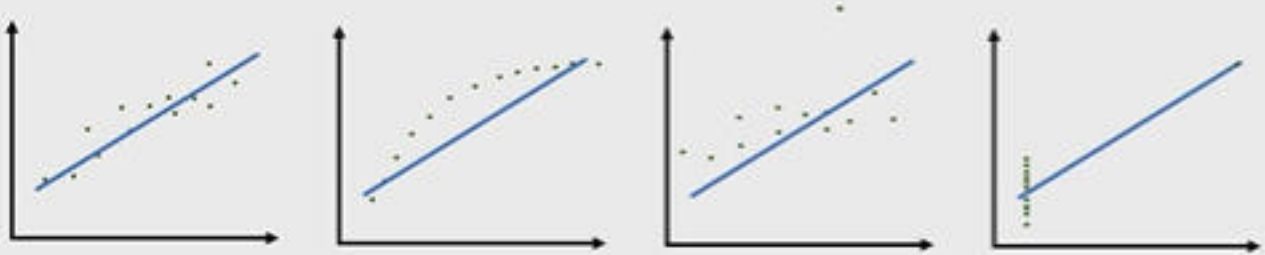
R^2 can be misleading. The following all have the same best fit line:



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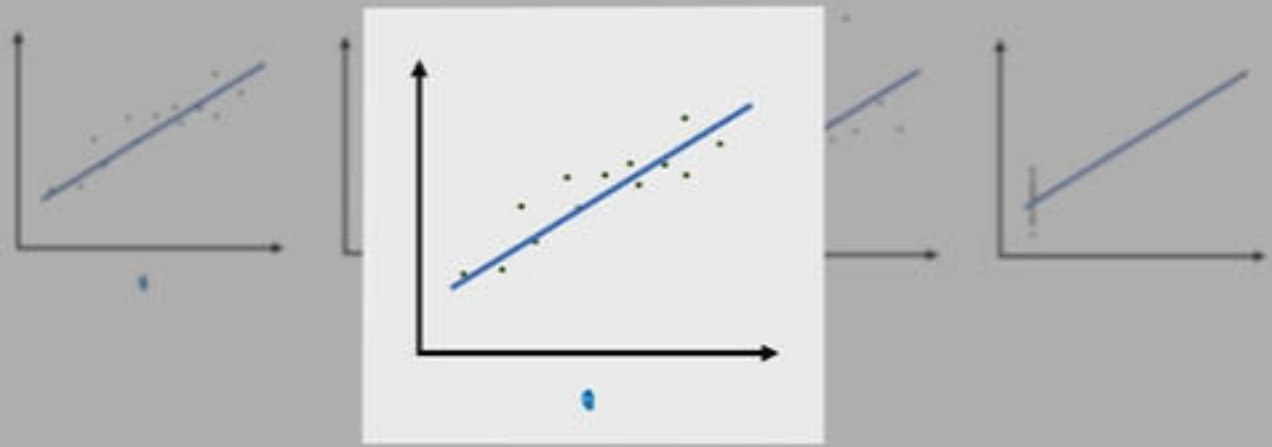

Extending to Many Variables

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Data matrix

$i = 1, \ldots, N$

$\vec{x}_i = [x_{i1}, x_{i2}, \ldots, x_{iM}]$ ← M features

indep var.

y_i ← dep variable

data

X

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Extending to Many Variables

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Data matrix $i = 1, \ldots, N$

$\vec{x}_i = [x_{i1}, x_{i2}, \ldots, x_{iM}]$ ← M features

indep var.

y_i ← dep variable

$\underline{\text{Lin}}$

$y = \underline{a}x + \underline{b}(i)$

data matrix, X =

$$\begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1M} \\ \vdots & \vdots & \ddots & & \vdots \\ 1 & x_{N1} & x_{N2} & \cdots & x_{NM} \end{bmatrix}$$

$$\hat{y}_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_M x_{iM} =$$

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Extending to Many Variables

The loss function

$$\min L = \sum_{i=1}^{N} \left(y_i - \hat{y}_i \right)^2$$

$$= \sum_{i=1}^{N} \left(y_i - \left(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_M x_{iM} \right) \right)^2$$

$$= \sum_{i=1}^{N} \left(y_i - \vec{x}_i \cdot \vec{\beta} \right)$$

Extending to Many Variables

aws training and certification

The loss function

$\underline{\min L}$

$$L = \sum_{i=1}^{N} \left(y_i - \hat{y}_i \right)^2$$

$$= \sum_{i=1}^{N} \left(y_i - \left(\beta_0 + \beta_1 x_{i1} + \dots + \beta_M x_{iM} \right) \right)^2$$

$$= \sum_{i=1}^{N} \left(y_i - \vec{x}_i \cdot \vec{\beta} \right)^2$$

$$= \|$$

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Extending to Many Variables

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The loss function

min

$$L = \sum_{i=1}^{N} \left(y_i - \hat{y}_i \right)^2$$

$$= \sum_{i=1}^{N} \left(y_i - \left(\beta_0 + \beta_1 x_{i1} + \dots + \beta_M x_{iM} \right) \right)^2$$

$$= \sum_{i=1}^{N} \left(y_i - \vec{x}_i \cdot \vec{\beta} \right)^2$$

$$= \| \vec{y} - X\vec{\beta} \|_2^2$$

$\| \cdot \|_2 \rightarrow$ L2 norm of vec

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Extending to Many Variables

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The loss function

min L

$$L = \sum_{i=1}^{N} \left(y_i - \hat{y}_i \right)^2$$

$$= \sum_{i=1}^{N} \left(y_i - \left(\beta_0 + \beta_1 x_{i1} + \dots + \beta_M x_{iM} \right) \right)^2$$

$$= \sum_{i=1}^{N} \left(y_i - \vec{x}_i \cdot \vec{\beta} \right)^2$$

$$= \| \vec{y} - X\vec{\beta} \|_2^2$$

$\| \cdot \|_2 \rightarrow$ L2 norm of vector.

$$= (y - X\beta)^T (\cdot$$

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A Few Facts from Matrix Calculus

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$$\frac{\partial[X\vec{\beta}]}{\partial\vec{\beta}} = X^T \longleftrightarrow \frac{d(ax)}{dx} = a$$

$$\frac{\partial[\vec{\beta}^T A\vec{\beta}]}{\partial\vec{\beta}} = 2A^T\vec{\beta} \qquad \frac{d(ax^2)}{dx}$$

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Minimizing the Loss

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$$L = (y - X\beta)^T (y - X\beta)$$

$$\frac{dL}{d\beta} = 0 \Rightarrow \frac{d}{d\beta}($$

-2:49

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Minimizing the Loss

aws training and certification

$$L = (y - X\beta)^T (y - X\beta)$$

$$\frac{dL}{d\beta} = 0 \Rightarrow \frac{d}{d\beta}\left((y - X\beta)^T (y - X\beta)\right) = 0$$

$$\Rightarrow \frac{d}{d\beta}\left(\underbrace{y^T y}_{0} - \underbrace{y^T X\beta} - \underbrace{\beta^T X^T y} + \underbrace{\beta^T X^T X\beta}\right) = 0$$

$$\Rightarrow -(X^T y) - (X^T y) + 2(X^T X)\beta = 0$$

$$\left((XY)^T = Y^T X^T \right)$$

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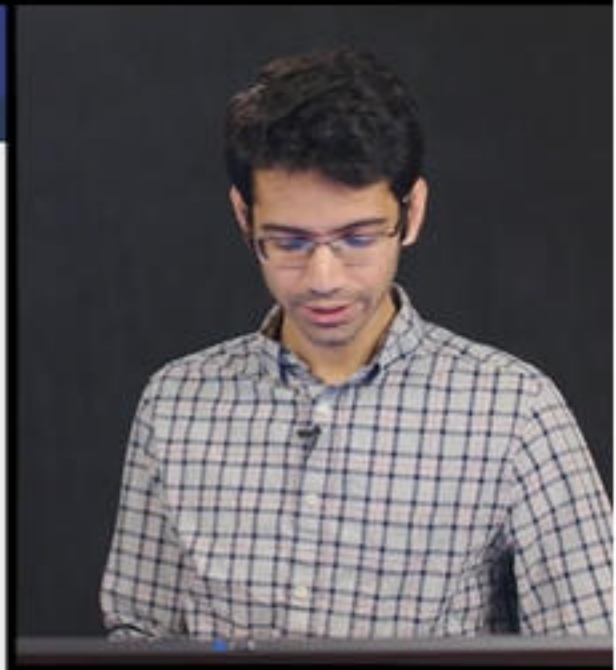

-1:14

OLS Pros

- Efficient computation ✓
- Unique minimum ✓
- Stable under perturbation of data ✓
- Easy to interpret ✓

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OLS Cons

- Influenced by outliers
- $(X^T X)^{-1}$ need not exist

X cols/features are lin. indep.

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Maximum Likelihood Estimate (MLE)

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- Review: Maximum Likelihood Estimates
- A Note on Logarithms
- Definition
- Goal
- A Significant Issue

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Minimize MSE $\Leftrightarrow$ MLE

- Relation to the Previous Problem
- Solution (As Seen Last Time)

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Maximum Likelihood Estimate (MLE)

This video looks at OLS and loss function under a probabilistic light. The video also reviews MLE but first, take a moment to consider the following:

In an OLS model, the choice of least squares is arbitrary.

Why are we only choosing the power of 2, and not the sum of cubes or other degree values?

$$L = \sum_{i=1}^{n} (y_i - \bar{y}_i)^2$$

$$\hat{\theta} = \underbrace{arg}_{\theta} \underbrace{max\ L(\theta; Y)}_{\theta \text{ that maximizes L}}$$

Viewing OLS in a Probabilistic Light

$$L = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

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Viewing OLS in a Probabilistic Light

$$L = \sum_{i=1}^{N} \left(y_i - \hat{y}_i \right)^2$$

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Viewing OLS in a Probabilistic Light

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$$L = \sum_{i=1}^{N} (Y_i - \hat{Y}_i)^2$$

arbitrary?

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Review: MLE

We will review MLE using the example of coin flips.

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$p \leftarrow$ heads probability

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Review: MLE

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$p \leftarrow$ heads probability

$\{HTHHHT\}$

$$P(Y) = P(\{HTHHHT\})$$
$$= P(H)P(T)P(H)P(H)P(H)P(T)$$
$$= p^4(1-p)^2$$

$$\left(\begin{aligned} P(E_1 E_2) &= P(E_1)P(E_2) \end{aligned} \right)$$

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$$\left(P(E_1 E_2) = P(E_1)P(E_2) \right)$$

$$L = \underbrace{p^4(1-p)^2}$$

$$\frac{dL}{dp} = 0 \Rightarrow 2\cancel{p^3}(1-p)^2 + 2p^{\cancel{4}}(\cancel{1-p})(-1) = 0$$

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$$\frac{dL}{dp} = 0 \Rightarrow 2\cancel{p^3}(1-p)^2 + 2p^4(\cancel{1-p})(-1) = 0$$

$$2(1-p) - p = 0$$

$$\Rightarrow \boxed{p = 2/3}$$

-4:31

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A Note on Logarithms

In probability, probabilities of independent events **multiply**. This means likelihoods of data is often a **giant product**.

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In probability, probabilities of independent events **multiply**. This means likelihoods of data is often a **giant product**.

$$\log(AB) = \log A + \log B$$

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In probability, probabilities of independent events **multiply**. This means likelihoods of data is often a **giant product**.

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A Note on Logarithms

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$$\log(AB) = \log A + \log B$$

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-2:40

A Note on Logarithms

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Definition

MLE . $\hat{\theta} = \arg\max$

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Definition

MLE . $\hat{\theta} = \arg\max_{\theta} L(\theta; Y)$

θ maximize

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Definition

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MLE . $\hat{\theta} = \arg\max_{\theta} L(\theta; Y)$

$\theta \rightarrow$ maximize

$= \mathbb{P}(\{Y_i ; i=1 \dots N\} \mid \theta$

-1:15

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Definition

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MLE . $\hat{\theta} = \arg\max_{\theta} L(\theta; Y)$

$\theta \rightarrow$ maximize

$= \mathbb{P}_{\theta}(\{Y_i ; i=1 \dots N\})$

-1:05

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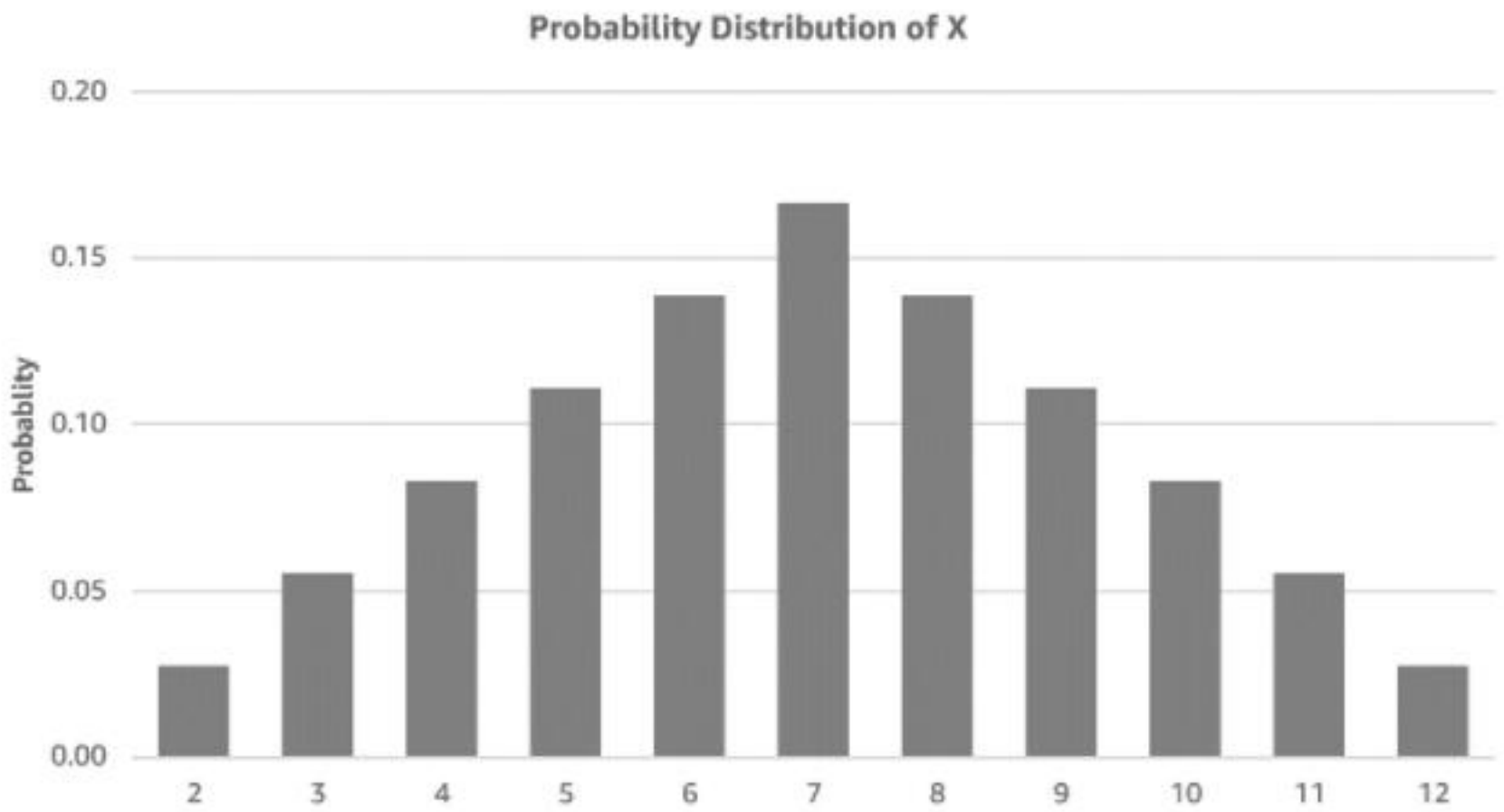
Continuous Probability

In this video, we'll explore continuous probability and common types of these random variables.

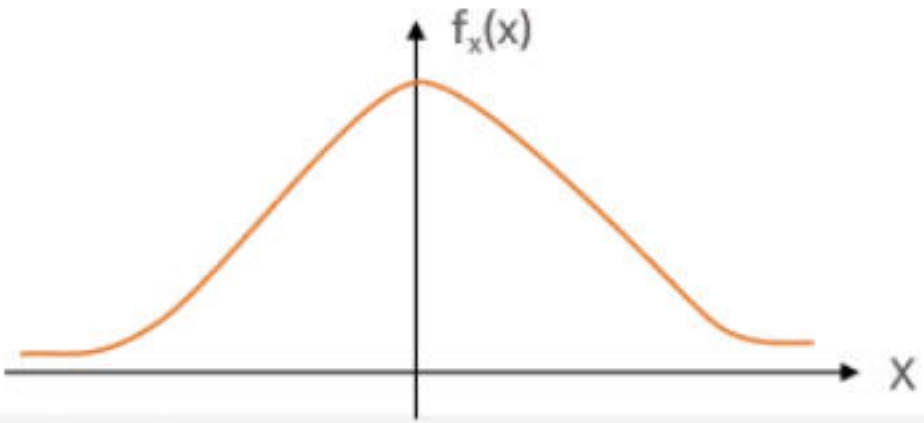
Discrete Random Variables:

Sum of two dice



Continuous Random Variable:

Probability density function



$$X \sim Gaussian\left(\mu, \sigma^2\right) \sim \mathcal{N}\left(\mu, \sigma^2\right)$$

$$f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{(x-\mu)^2}{2\sigma^2}}$$

Where
μ - mean of probability density function
Σ – standard deviation

A Significant Issue

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With continuous variables, you can no longer just use probability (the probability a Gaussian is equal to 2.317635618… is 0). Therefore, you need to expand your point of view to **densities**.

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Definitions

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Probability Density Function

$f_X(x)$

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Definitions

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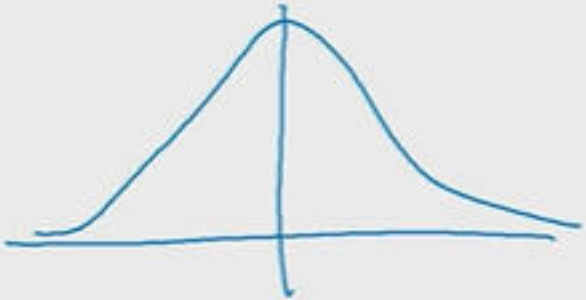
Gaussian Random Variables



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Definitions

Gaussian Random Variables

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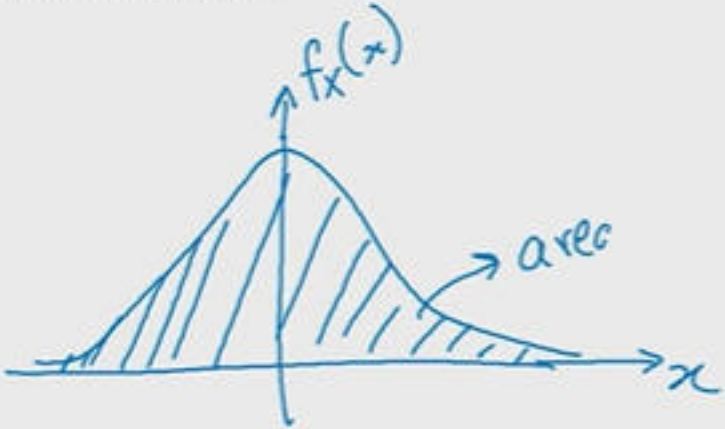
Definitions

Gaussian Random Variables



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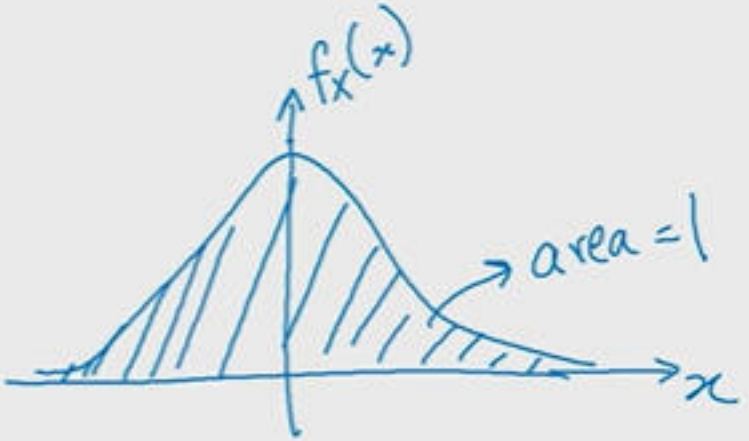
Definitions

Gaussian Random Variables

$$f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



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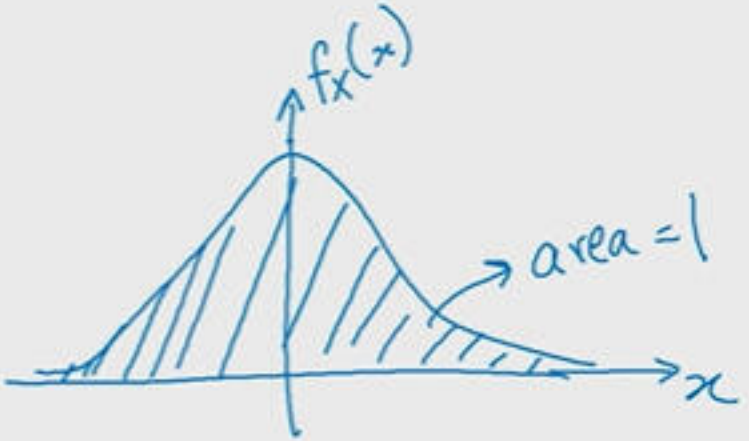

μ, σ

mean

standard deviation

(σ^2 ← variance)

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Definitions

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Gaussian Random Variables

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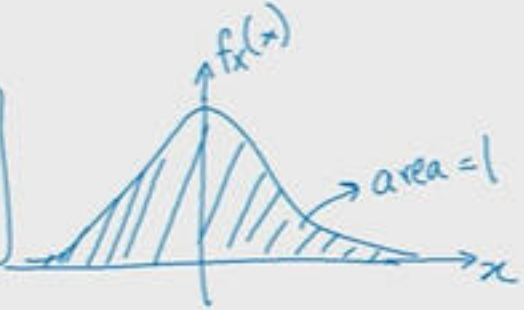

μ, σ

mean

standard deviation

($\sigma^2 \leftarrow$ variance)

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Idea

We now extend MLE to **densities** rather than probabilities.

$$L(\theta) = P_\theta(\{Y_i : i=1,\dots,N\})$$

$$\updownarrow$$

cont. RV.

$$L(\theta) = f_X(\{Y_i : i=1,\dots,N\})$$

$$= \prod_{i=1} f_X(Y_i)$$

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$$L(\theta) = P_\theta(\{Y_i : i=1,\dots,N\})$$

cont. RV.

$$L(\theta) = f_X(\{Y_i : i=1,\dots,N\})$$

$$= \prod_{i=1}^{N} f_X(Y_i)$$

$$\boxed{\log L(\theta) = \sum_{i=1}^{N} \log f_X(y_i)}$$

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-0:02

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Gaussian Maximum Likelihood Estimate (MLE)

-5:52

Example

Suppose we want to find the MLE for μ when $x \sim \mathbf{N}\ (\mu, 1)$ given observations: $x_1, x_2, x_3 \ldots \ldots x_n$

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Example

Suppose we want to find the MLE for μ when $x \sim \mathbf{N}\ (\mu, 1)$ given observations: $x_1, x_2, x_3 \ldots \ldots x_n$

$$f_X(x) = \left(\frac{1}{\sqrt{2\pi}}\right)\exp\left(-\frac{(x-\mu)^2}{2}\right) \Rightarrow \log f_X(x) = -\frac{1}{2}\log(2\pi) - \frac{(x-\mu)^2}{2}$$

$$\log(L) = \sum_{i=1}^{n} \log f_X(x_i) = -\frac{n}{2}\underbrace{\log(2\pi)}_{0} - \frac{1}{2}\sum_{i=1}^{n}(x_i-\mu)^2$$

$$\text{MLE}, \hat{\mu} : \frac{d(\log)}{d\mu} = 0 \Rightarrow \sum_{i=1}^{n}(x_i-\hat{\mu})(-1) = 0$$

$$\Rightarrow \boxed{\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i}$$

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A Note

We see here that **maximum** likelihood estimation is equivalent to **minimizing** the sum of squared errors.

$$\frac{dL}{d\mu} = 0$$

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$$\frac{dL}{d\mu} = 0 \Rightarrow \frac{d}{d\mu}\left(-\sum_{i=1}^{n}(x_i-\mu)^2\right) = 0$$

maximize L = minimize sum of squared errors.

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Topics

- OLS as MLE
- The Model

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OLS AS MLE

We can now **rephrase** OLS as a **likelihood maximization problem**.

OLS:

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OLS AS MLE

We can now **rephrase** OLS as a **likelihood maximization problem**.

OLS:

$$\begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix} = \bar{y} = X\bar{\beta}$$

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output variable. data matrix coefficients

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OLS AS MLE

We can now **rephrase** OLS as a **likelihood maximization problem**.

OLS:

$$\begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix} = \hat{\bar{y}} = X\bar{\beta}$$

output variable

data matrix

coefficients

$$\bar{y} = X\bar{\beta} + \epsilon$$

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OLS:

$$\begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix} = \underbrace{\hat{\bar{y}}}_{\text{output variable}} = \underbrace{X}_{\text{data matrix}} \underbrace{\bar{\beta}}_{\text{coefficients}}$$

$$\bar{y} = X\bar{\beta} + \underline{\epsilon}$$

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The Model

$$\epsilon \sim N(0, \sigma^2)$$

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Likelihood of Given Data

μ

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Likelihood of Given Data

$y_i \sim N(\bar{x}_i \cdot \bar{\beta}, \sigma^2) \longleftrightarrow \bar{y} \sim$

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Likelihood of Given Data

$$y_i \sim N(\bar{x}_i \cdot \bar{\beta}, \sigma^2) \longleftrightarrow \bar{y} \sim N(X\bar{\beta}, \Sigma^2)$$

$$f_Y(y_i, \underline{x}_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp($$

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Likelihood of Given Data

$$y_i \sim N(\bar{x}_i \cdot \bar{\beta}, \sigma^2) \longleftrightarrow \bar{y} \sim N(X\bar{\beta}, \Sigma^2)$$

$$f_Y(y_i, x_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - \bar{x}_i \cdot \bar{\beta})^2}{2\sigma^2}\right)$$

$$\log f_Y(y_i, x_i) = -\frac{1}{2}\log(2\pi\sigma^2) - \frac{(y_i - \bar{x}_i \cdot \bar{\beta})^2}{2\sigma^2}$$

$$L(\beta, \sigma^2) = \sum_{i=1}^{N}$$

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Likelihood of Given Data

$$y_i \sim N(\bar{x}_i \cdot \bar{\beta}, \sigma^2) \longleftrightarrow \bar{y} \sim N(X\bar{\beta}, \Sigma^2)$$

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$$\log f_Y(y_i, x_i) = -\frac{1}{2}\log(2\pi\sigma^2) - \frac{(y_i - \bar{x}_i \cdot \bar{\beta})^2}{2\sigma^2}$$

$$L(\beta, \sigma^2) = \sum_{i=1}^{N} \left(\log f_Y(y_i | x_i)\right)$$

$$= -\frac{N}{2}\log(2\pi\sigma^2) - \sum_{i=1}^{N} \frac{(y_i - \bar{x}_i \cdot \bar{\beta})^2}{2\sigma^2}$$

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Likelihood in Matrix Form

$$\log L(\beta, \sigma^2) = -\frac{1}{2\sigma^2} \|\bar{y} - X\bar{\beta}\|_2^2 - \frac{1}{2} \log(2\pi\sigma^2)$$

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Relation to the Least Squares Approach

$$\log L(\beta, \sigma^2) = -\frac{N}{2}\log(\cancel{2\pi}\sigma^2) - \frac{1}{2}\underbrace{(\bar{y} - X\bar{\beta})^T(\bar{y} - X\bar{\beta})}$$

$$\frac{d}{d\beta}\log L = 0$$

$$\Rightarrow \frac{d}{d\beta}\left(-\frac{1}{2}\underbrace{(\bar{y} - X\bar{\beta})^T(\bar{y} - X\bar{\beta})}_{\text{MSE}}\right) = 0$$

MLE

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Solution

Suppose we model our problem as:

$$y \sim \vec{x}\vec{\beta} + \mathcal{N}(0, \sigma^2).$$

Then, the maximum likelihood estimate of $\vec{\beta}$ is

$$\hat{\beta} = (X^T X)^{-1} X^T \vec{y},$$

same as MSE approach.

the same as the OLS estimator

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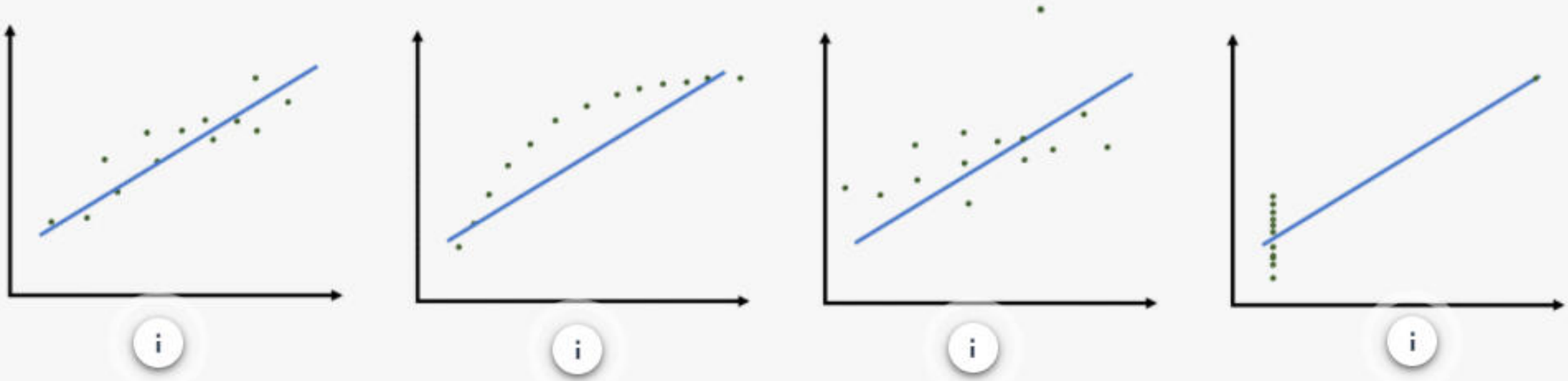
Improvement #1

Event 1 Title

This lets you get the MLE for standard deviation (\sigma).

$$\sigma^2 = \frac{2\pi}{N} \left\| \bar{Y} - X\bar{\beta} \right\|_2^2$$

Improvement in Anscombe's Quartet



First Upshot

We can get a MLE for σ.

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First Upshot

We can get a MLE for σ.

$$\log \mathcal{L} = -\frac{1}{2\sigma^2} \|\bar{y} - X\bar{\beta}\|_2^2 - \frac{N}{2} \log(2\pi\sigma^2)$$

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First Upshot

We can get a MLE for σ.

$$\log \mathcal{L} = -\frac{1}{2\sigma^2} \|\bar{y} - X\bar{\beta}\|_2^2 - \frac{N}{2} \log(2\pi\sigma^2)$$

$$\frac{\partial \log \mathcal{L}}{\partial \sigma} = \frac{\|\bar{y} - X\bar{\beta}\|_2^2 (2)}{2\sigma^3} - \frac{N}{2} \frac{1}{2\pi\sigma^2} (2\pi\sigma)(2)$$

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First Upshot

We can get a MLE for σ.

$$\log \mathcal{L} = -\frac{1}{2\sigma^2}\|\bar{y} - X\bar{\beta}\|_2^2 - \frac{N}{2}\log(2\pi\sigma^2)$$

$$\frac{\partial \log \mathcal{L}}{\partial \sigma} = \frac{\|\bar{y} - X\bar{\beta}\|_2^2 (\cancel{2})}{\cancel{2}\sigma^3} - \frac{N}{\cancel{2}}\frac{1}{\cancel{2}\cancel{\pi}\sigma^{\cancel{2}}}(\cancel{2}\cancel{\pi}\cancel{\sigma})(\cancel{2}) =$$

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Summary

Thus, we may interpret the MSE loss function as a MLE for the variance of the Gaussian noise.

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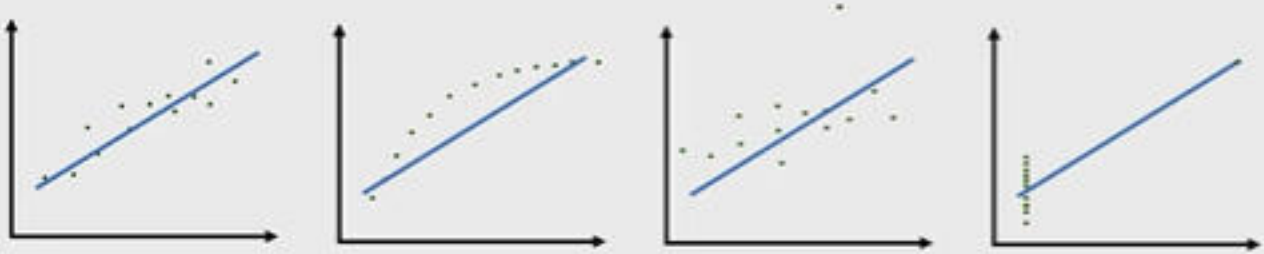
Second Upshot

We may gain a deeper understanding of Anscombe's Quartet.



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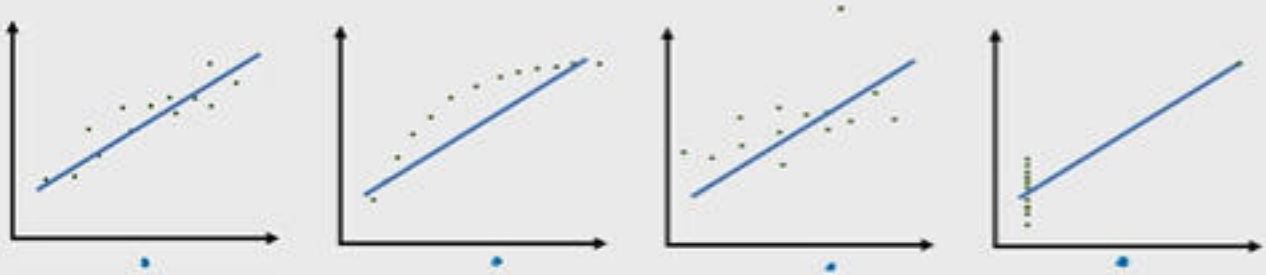

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Second Upshot

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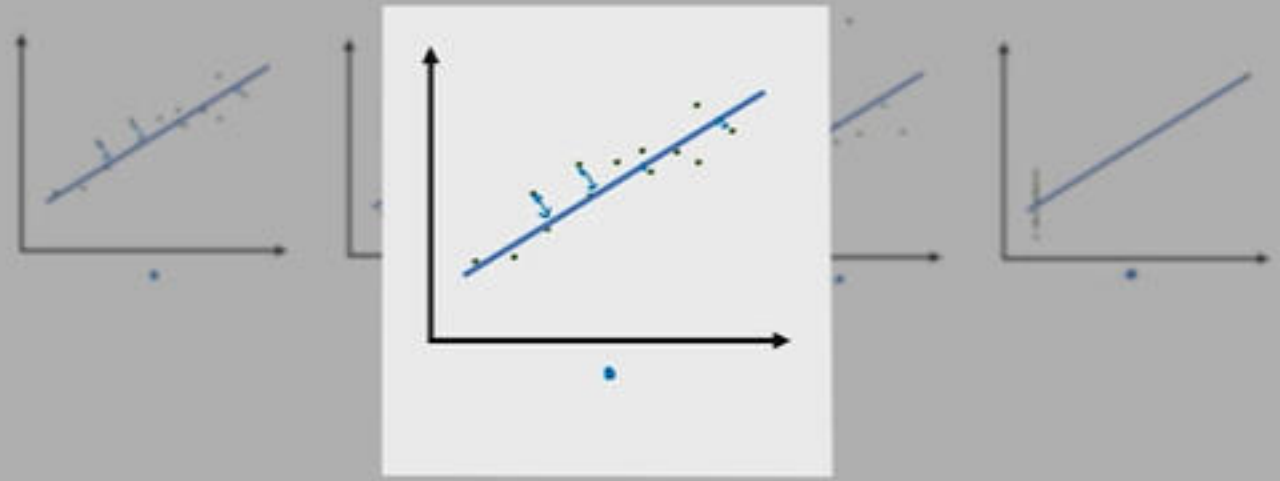
We may gain a deeper understanding of Anscombe's Quartet.



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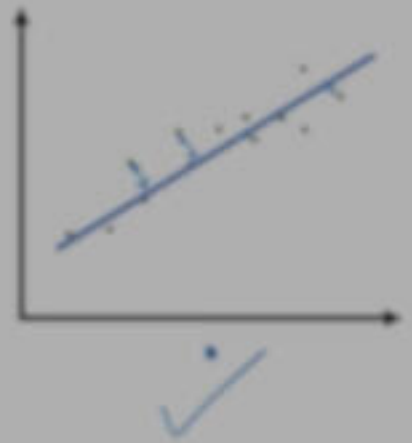
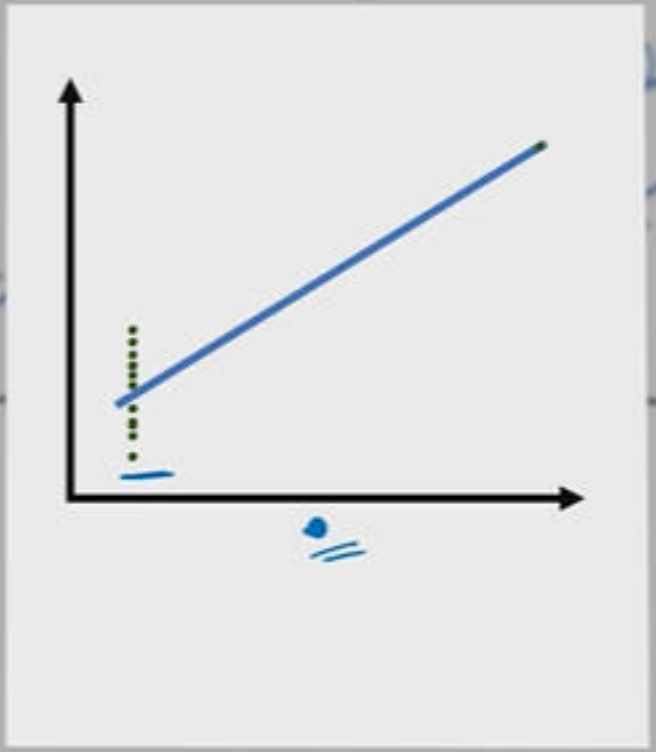
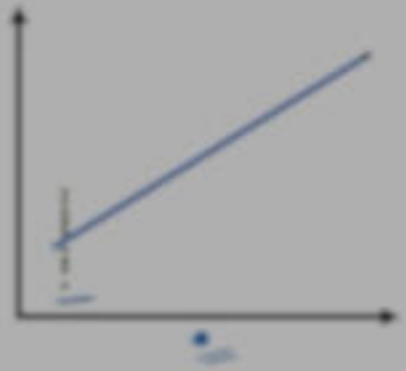
We may gain a deeper understanding of Anscombe's Quartet.







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Third Upshot

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Prediction Improvement

① Error model is not correct → Different error model.

② Error not indep. w/ x → Tva

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Assumptions of OLS, Nonlinear OLS, Regularization, and Cross-Validation

Introduction

This video contains lessons as they relate to the assumptions of linear regression, overfitting an
regularization.

The following topics will be covered:

- Assumptions of linear regression
- Concept of residuals
- Extensions of linearity
- Extreme learning machines
- Overfitting
- Regularizations
- Other issues

Extensions of Linear Regression

- Extensions of Linear Regression

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Beyond Linearity

- Definition
  - Residuals
- Assumptions on Residuals
- A Good Residual Plot
- A Bad Residual Plot
- OLS Actually Applies Beyond Linear Models
- Basis Functions

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Regularization

- The Bayesian Point of View
- Ridge Regression
- LASSO Regression
- The Geometry of Regularization
- The Geometry of Ridge Regularization
- The Geometry of LASSO Regularization
- Elastic Net Regression

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Assumptions of Linear Regression

In the linear regression model, various assumptions were made. This video covers how the model performs outside of those assumptions. The assumptions made in a linear regression model are:

Model

Click to flip

Errors

X^TX

Assumptions of Linear Regression

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1. Linearity

$$\bar{y} = X\bar{\beta} + N(0, \Sigma)$$

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Assumptions of Linear Regression

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2. The errors are independent normals

$$\underbrace{N}_{\text{normal}}\left(\underbrace{0}_{\cdot 2}, \Sigma^2\right)$$

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Assumptions of Linear Regression

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2. The errors are independent normals

$$\underbrace{N}_{\text{normal}}\left(\underbrace{0}_{\text{zero mean}}, \underbrace{\Sigma^2}_{\text{covariance matrix}}\right) \text{ (diagonal)} \quad \begin{bmatrix} \sigma^2 & & 0 \\ & \sigma^2 & \\ 0 & & \ddots & \\ & & & \sigma^2 \end{bmatrix}$$

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Assumptions of Linear Regression

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3. $\boldsymbol{X^T X}$ is invertible

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

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Pushing Beyond Assumptions

We will continue to see how to **push beyond each of these assumptions**, one at a time, and see how **ordinary least squares** is actually far more **flexible** than usually assumed.

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Beyond Linearity

In this video, we discuss residuals and their plots, OLS models when the relationship between data matrix (X) and output function (Y) is nonlinear, and different basis functions that are used to expand features. Take a moment to explore residuals.

A residual plot:

Plot of ϵ against x.

Where

$$\epsilon_i = y_i(x) - \hat{y}_i$$

Assumptions:

Residuals are independent of x, normally distributed, and uncorrelated.

A good residual plot

Every creative endeavor requires that you take risks. If you try and don't succeed, you've still learned something. You're not failing. You're discovering what doesn't work.

A good residual plot

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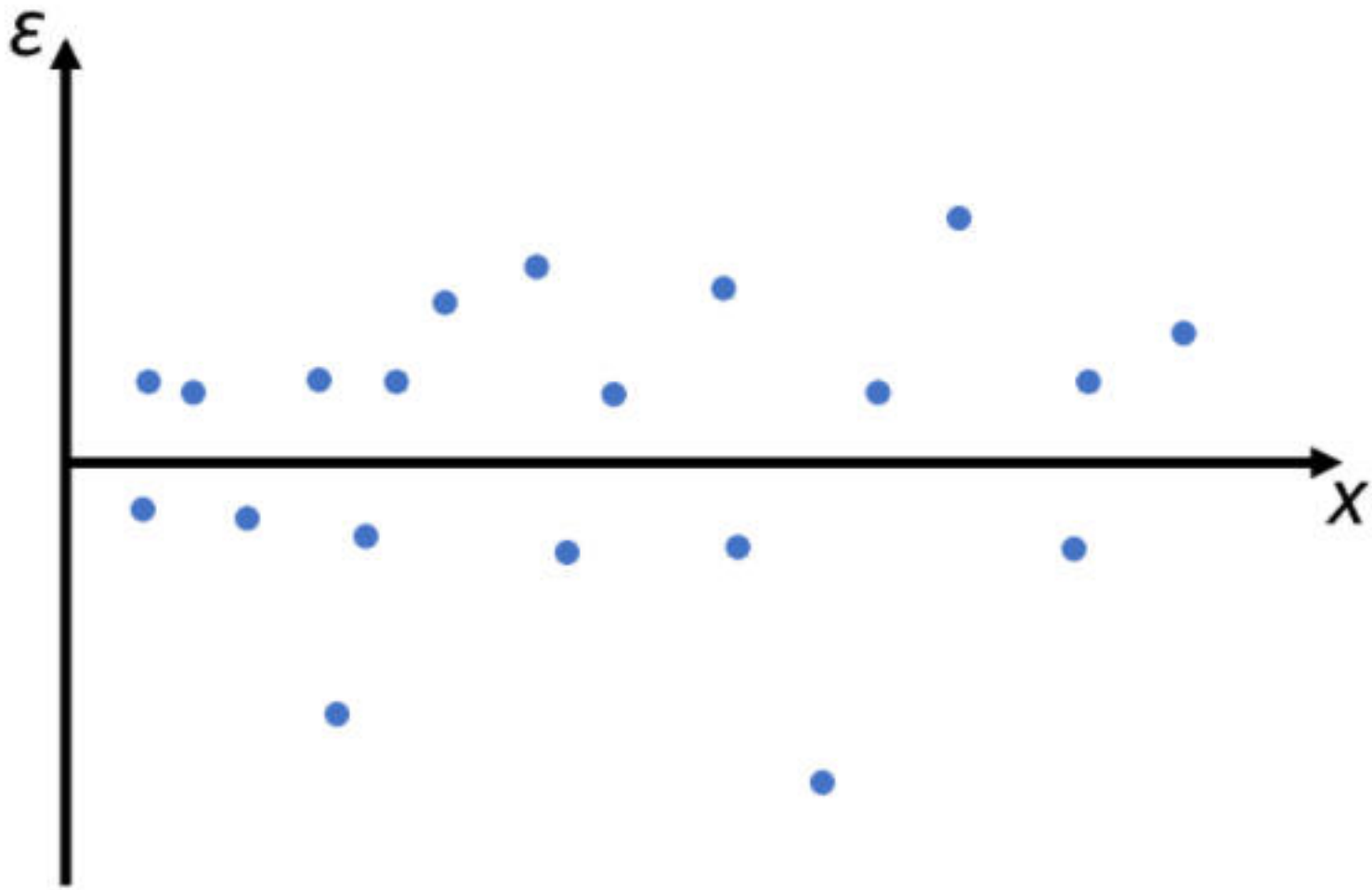
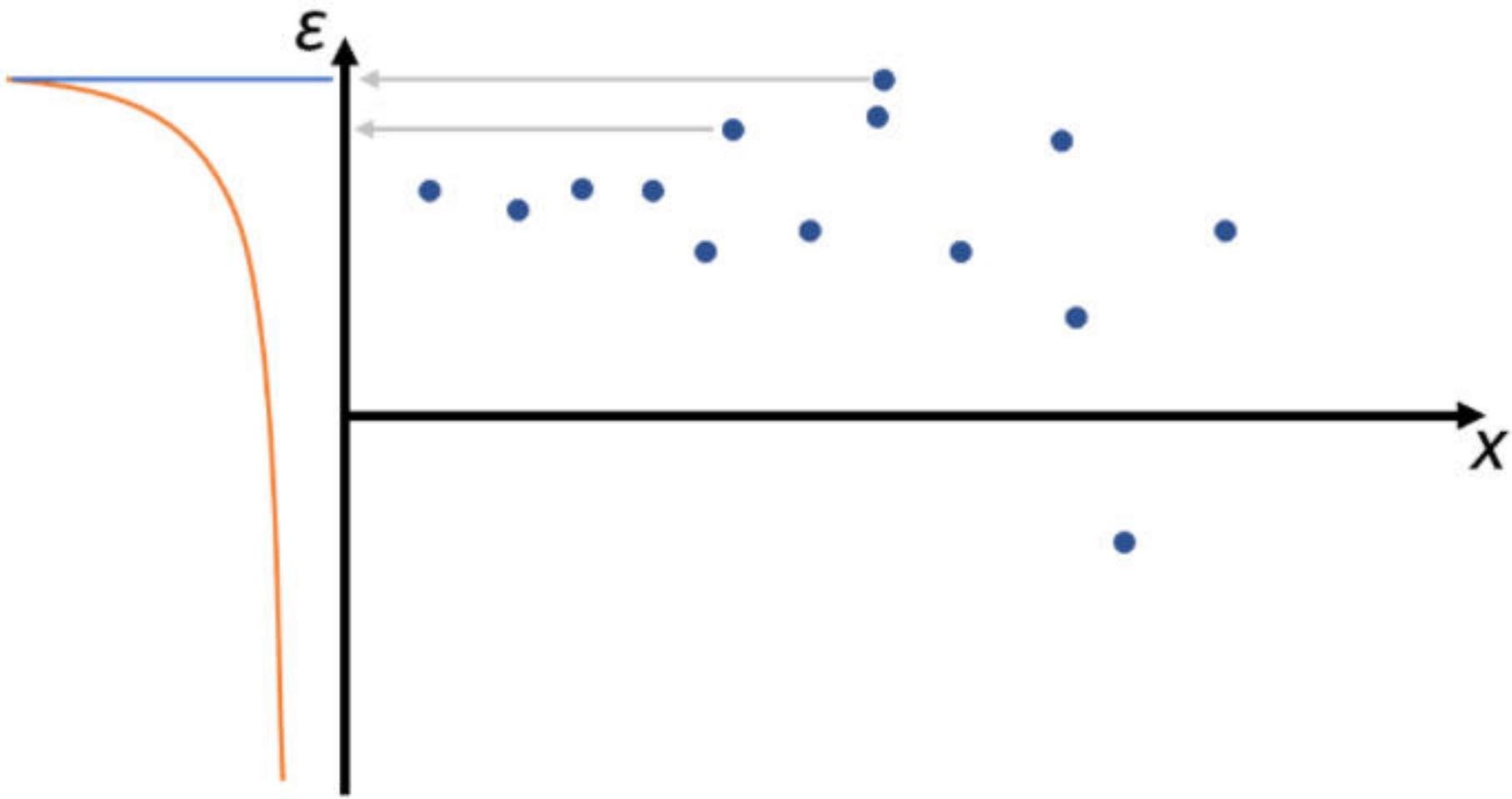


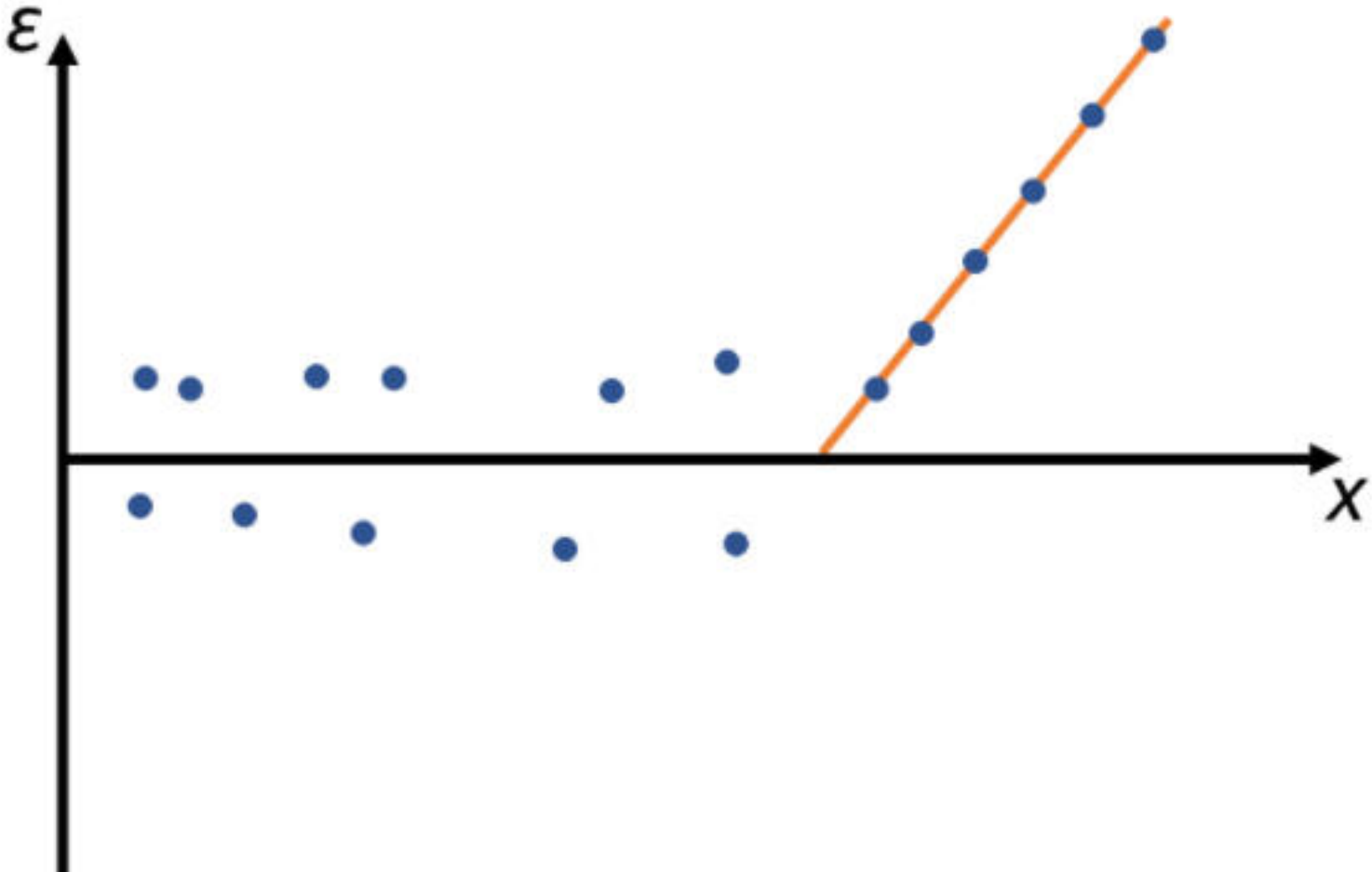
A bad residual plot

The errors are not normally distributed.



A misleading residual plot

Up to certain point the model seems to be a good fit, but after that the errors are dependent of variable x.



Topics

- Definition
  - Residuals
- Assumptions on Residuals
- A Good Residual Plot
- A Bad Residual Plot
- OLS Actually Applies Beyond Linear Models

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Definition

Residuals

$$\epsilon_i = y_i - \hat{y}_i$$

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Definition

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Residuals

$$\epsilon_i = y_i - \hat{y}_i$$

Residual plot

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Assumptions on Residuals

Assume the residuals are independent normals uncorrelated with x. If you plot (x_i, ϵ_i) pairs, then you can attempt to diagnose if this is a reasonable assumption.

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Assumptions on Residuals

Assume the residuals are independent, normals, uncorrelated with $\boldsymbol{x}$. If you plot (x_i, ϵ_i) pairs, then you can attempt to diagnose if this is a reasonable assumption.

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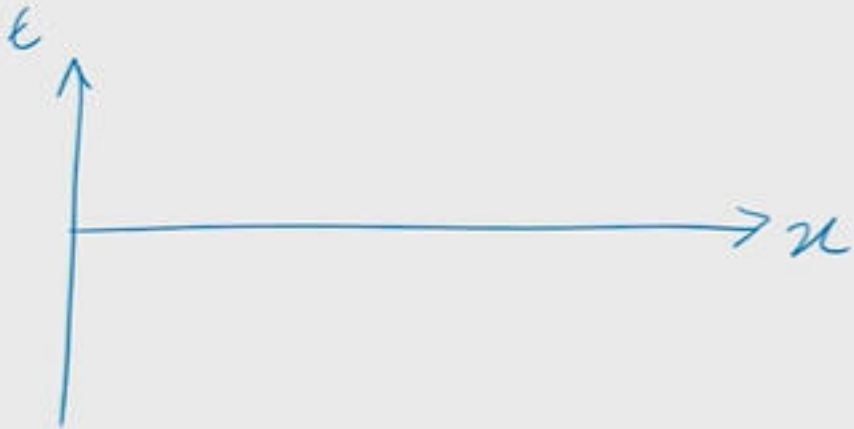
A Good Residual Plot



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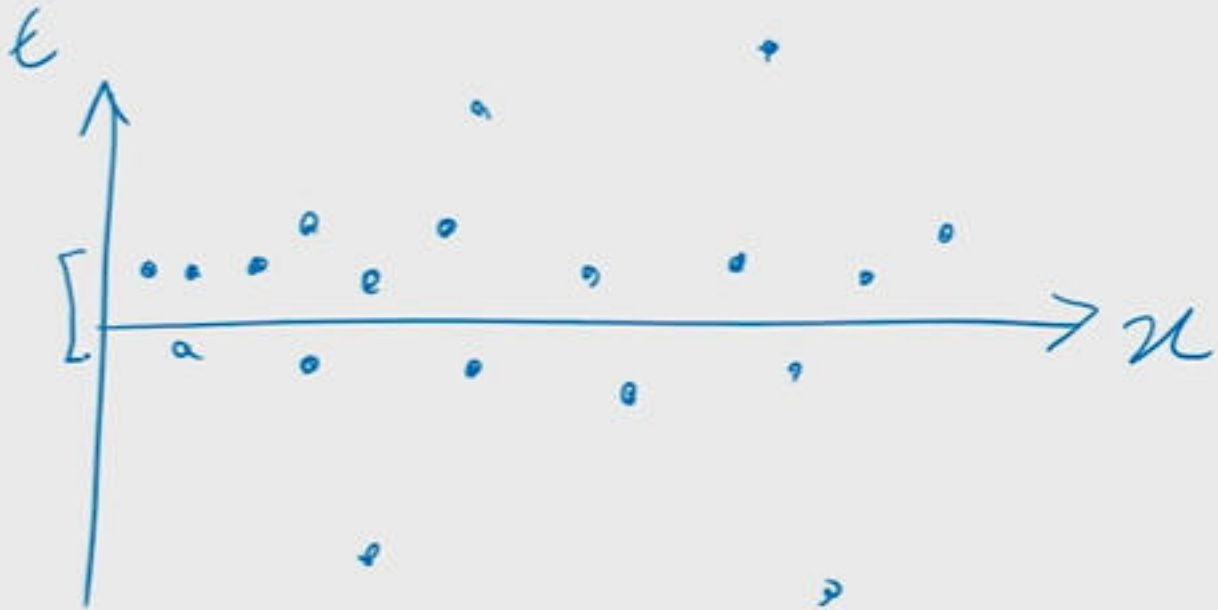
A Good Residual Plot



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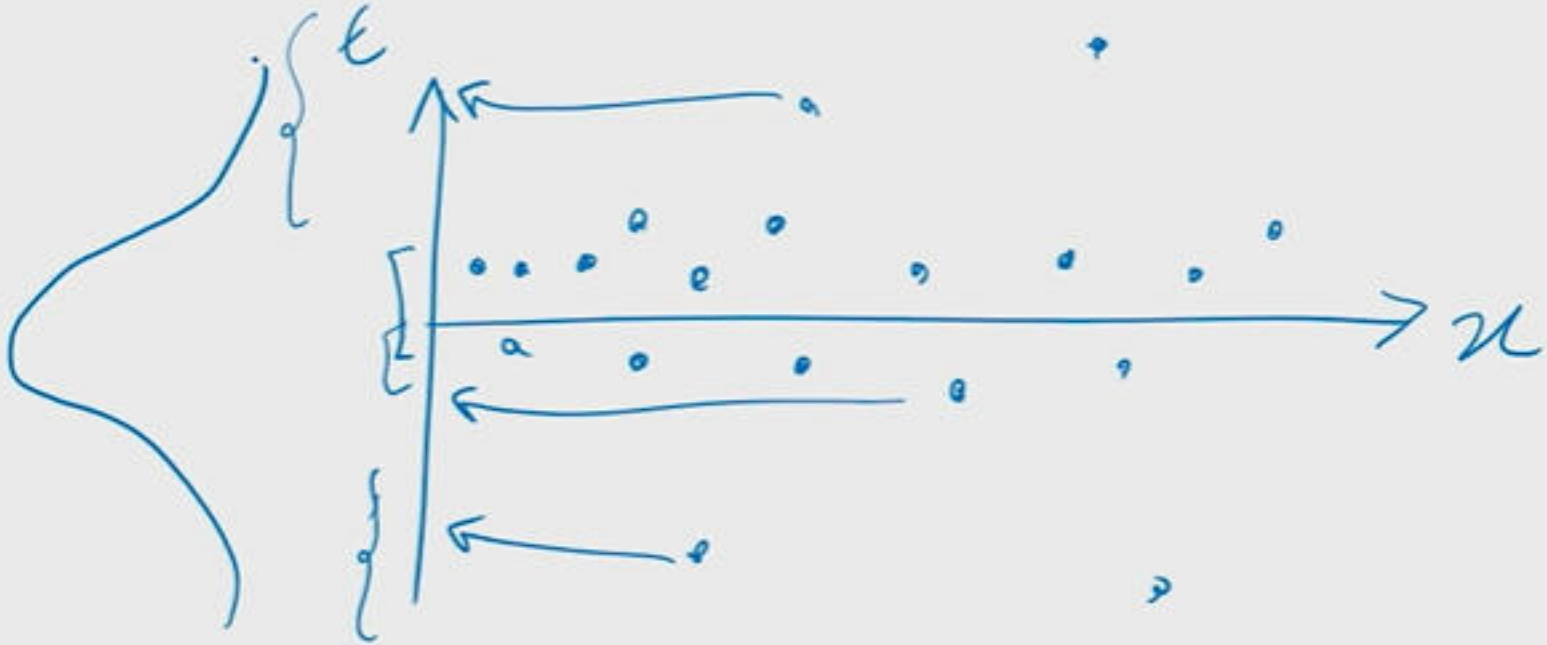

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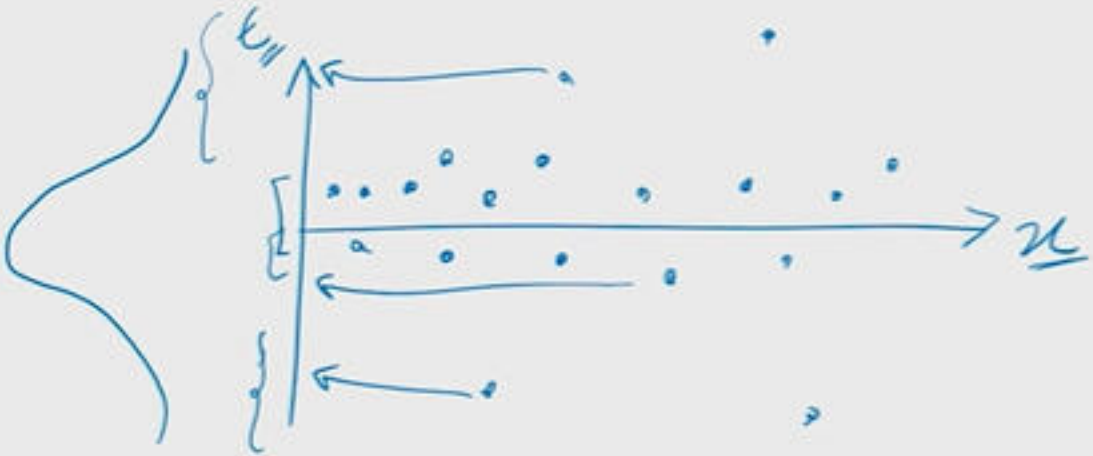
A Good Residual Plot



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A Bad Residual Plot

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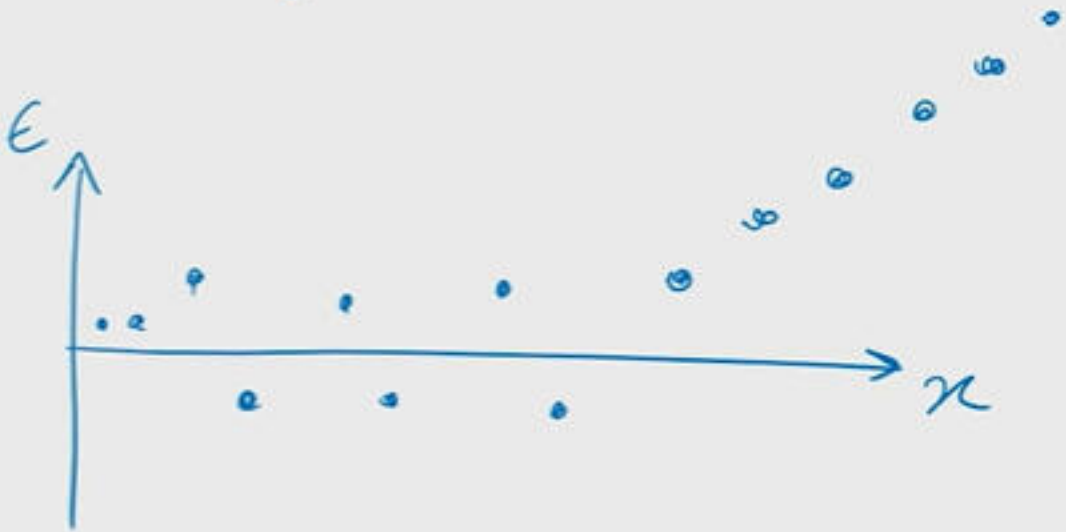

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Ordinary Least Squares (OLS) Applies Beyond Linear Models

You can augment your data matrix to use OLS to fit non-linear models:

$$y \sim \beta_0 \cdot 1 + \beta_1 x + \beta_2 x^2 + N(0,1)$$

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Ordinary Least Squares (OLS) Applies Beyond Linear Models

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	x	y
1	1	1·1
2	2	4·1
3	3	e
4	4	
⋮		

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	x	y
1	1	1.1
2	2	4.1
3	3	9.2
4	4	15.9
⋮		

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$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_n \end{bmatrix}$$

	x	y
0	1	1.1
1	2	4.1
2	3	9.2
3	4	15.9

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$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_N \end{bmatrix} \rightarrow \tilde{X} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_N & x_N^2 \end{bmatrix}$$

	x	y
①	1	1.1
②	2	4.1
③	3	9.2
④	4	15.9

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Basis Functions

You may use a basis function φ to expand our features with non-linear functions of the measured data in many ways. Here are a few common ones:

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Basis Functions

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You may use a basis function φ to expand our features with non-linear functions of the measured data in many ways. Here are a few common ones:

① polynomial $= (1, x, x^2, x^3, \dots, x^k)$

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② periodic $=$

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② periodic $= (1, \sin(x), \cos(x), \dots$

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③ ⊮

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Basis Functions

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② periodic $= (1, \sin(x), \cos(x), \sin(2x), \cos(2x), \ldots, \sin(kx), \cos(kx))$

③ kernel method $= (1, e^{-\|x - x_1\|^2},$

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Extreme Learning Machines

A particularly extreme version (circa 2006 or so) is to generate a large number of **random** non-linear features and use those.

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basis functions = (1, x,

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Extreme Learning Machines

A particularly extreme version (circa 2006 or so) is to generate a large number of **random** non-linear features and use those.

$$\text{basis functions} = \left(1, x, \tan^{-1}(x \cdot w_1), \tan^{-1}(x \cdot w_2), \ldots, \tan^{-1}(\vec{x} \cdot \vec{w}_k)\right)$$

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$$\text{basis functions} = \left(1, \bar{x}, \tan^{-1}(\bar{x}\cdot\bar{\omega}_1), \tan^{-1}(\bar{x}\cdot\bar{\omega}_2), \ldots, \tan^{-1}(\bar{x}\cdot\bar{\omega}_k)\right)$$

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randomly generated vectors $\sim N(0, \xi)$

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randomly generated vectors $\sim N(0, \xi)$

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Performance

For a rough comparison, recall the MNIST digit recognition problem.

- Logistic regression gives about 92% accuracy.
- Most advanced neural networks give about 99.8% after days of training.

*Data Source: MNIST Database of Handwritten Digits

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Performance

For a rough comparison, recall the MNIST digit recognition problem.

- Logistic regression gives about 92% accuracy.
- Most advanced neural networks give about 99.8% after days of training.
- Extreme learning techniques give about 99.14% after a couple of **minutes**.

*Data Source: MNIST Database of Handwritten Digits

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Best Value For Your Time

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Opinion: Extreme learning machines are one of the best value for your time techniques in machine learning.

*Extreme learning machines: theory and applications (Huang, Shu, Siew) (2006)

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Best Value For Your Time

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Best Value For Your Time

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Opinion: Extreme learning machines are one of the best value for your time techniques in machine learning.

It is no harder than linear regression, but can often get within a handful of percent of the absolute best result.

Many people agree: the paper introducing it in 2006* has been cited nearly 5000 times.

*Extreme learning machines: theory and applications (Huang, Shu, Siew) (2006)

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References

- Huang, Guang-Bin; Zhu, Qin-Yu; Siew, Chee-Kheong (2006). "Extreme learning machine: theory and applications". Neurocomputing. 70 (1): 489–501. CiteSeerX 10.1.1.217.3692 Freely accessible. doi:10.1016/j.neucom.2005.12.126

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Dataset References

- Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. "Gradient-based learning applied to document recognition." Proceedings of the IEEE, 86(11):2278-2324, November 1998. Dataset available from http://yann.lecun.com/exdb/mnist/

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References

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Polynomial Regression of Different Degrees

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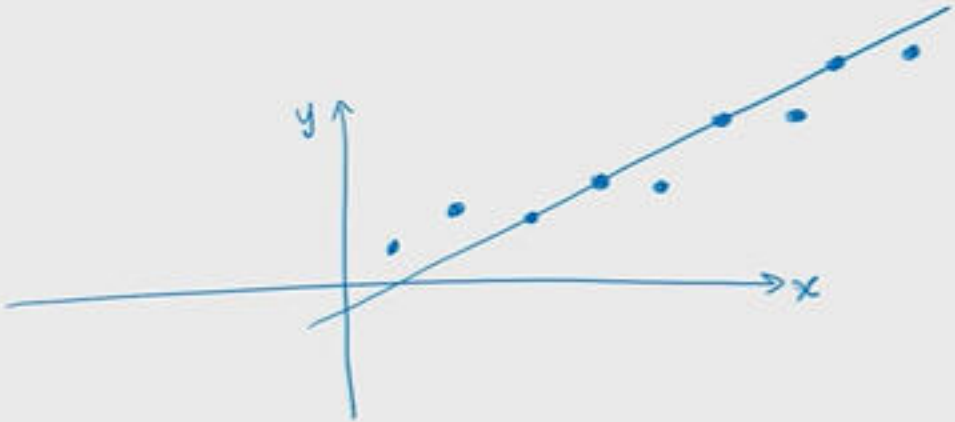
Polynomial Regression of Different Degrees



$y = ax + b$

$y = \beta_0 +$

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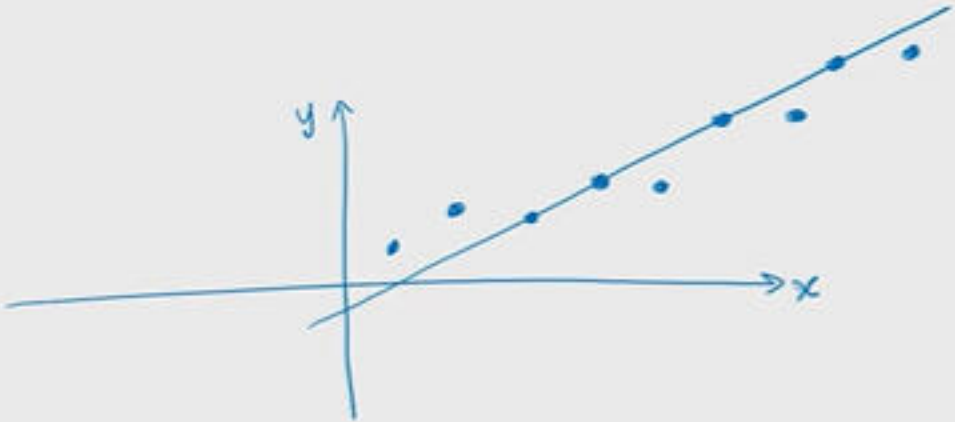
Polynomial Regression of Different Degrees



$$y = ax + b$$

$$y = \beta_0 + \beta_1 x + \beta_2 x^2$$

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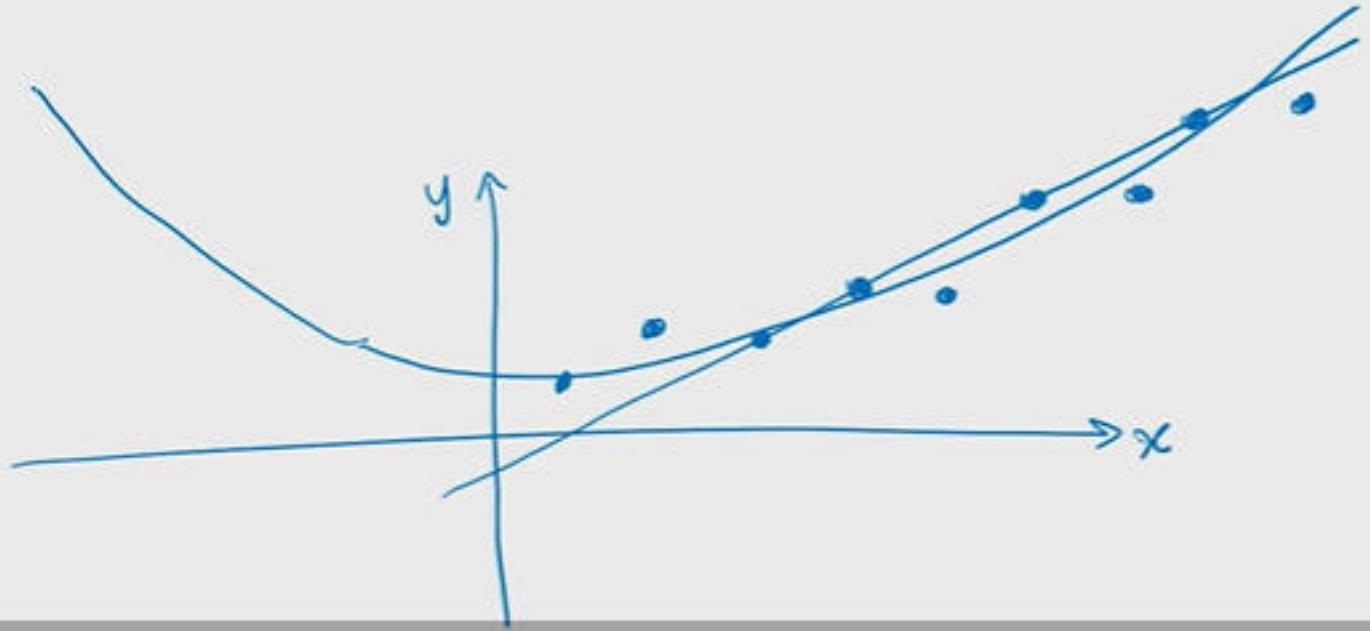
Polynomial Regression of Different Degrees



$$y = ax + b$$

$$y = \beta_0 + \beta_1 x + \beta_2 x^2$$

-1:51

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Polynomial Regression of Different Degrees

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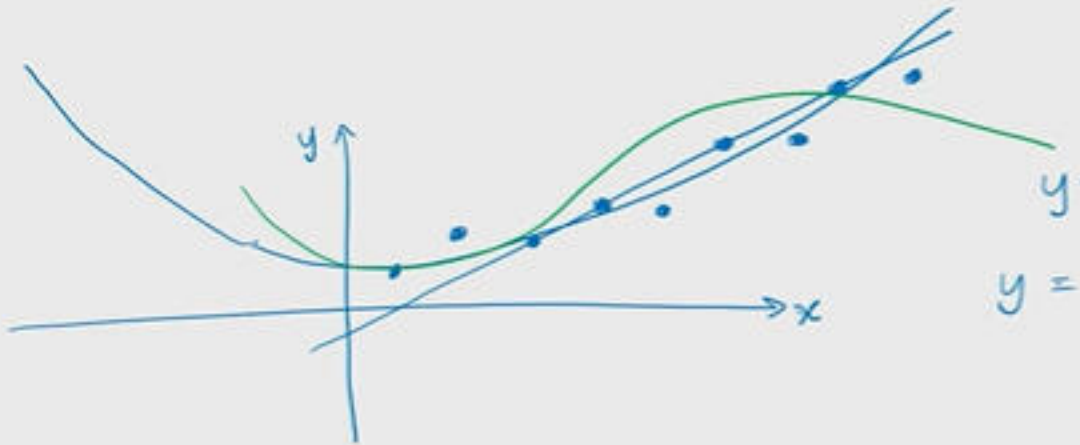

$y = ax + b$

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-1:24

Polynomial Regression of Different Degrees

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$y = ax + b$

$y = \beta_0 + \beta_1 x + \beta_2 x^2$

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-0:56

Polynomial Regression of Different Degrees

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The Solution: Regularization

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Regularization : penalize model complexity

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The Solution: Regularization

Regularization : penalize model complexity

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The Solution: Regularization

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The Solution: Regularization

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Regularization : penalize model complexity

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Regularization

Earlier when you computed the coefficients of linear model (ß) using MSE or MLE, you did not opt any model for ß. This was because you were unaware of the coefficients and didn't know of a model to represent them. Now, we'll explore regularization from the Bayesian point of view, learn how to obtain the model for ß using Ridge Regression and LASSO Regression techniques, and interpret the models using geometrical figures.

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Regularization

-20:30

Topics

- The Bayesian Point of View
- Ridge Regression
- LASSO Regression

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Topics

- The Bayesian Point of View
- Ridge Regression
- LASSO Regression
- The Geometry of Regularization
- The Geometry of Ridge Regularization
- The Geometry of LASSO Regularization

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- Elastic Net Regression

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The Bayesian Point of View

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MLE : $\bar{y} = X\bar{\beta} + N(0, \sigma^2)$

maximize $L(\beta)$: β^{MLE}

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The Bayesian Point of View

aws training and certification

MLE : $\bar{y} = \underbrace{X\bar{\beta}} + \underbrace{N(0, \sigma^2)} = N(X\bar{\beta}, \sigma^2)$

$\rightarrow$ $\underbrace{\text{maximize } L(\beta)}$: β^{MLE}

The Bayesian Point of View

MLE : $\underbrace{\bar{y}} = \underbrace{X\bar{\beta}} + \underbrace{N(0, \sigma^2)} = N(\underbrace{X}\bar{\beta}, \sigma^2)$

$\underbrace{\text{maximize } L(\beta)} : \beta^{MLE}$

$$L(\beta) = \prod_{i=1}^{N} f(X, Y \mid \underline{\beta})$$

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The Bayesian Point of View

MLE : $\underbrace{y} = \underbrace{X\bar{\beta}} + \underbrace{N(0, \sigma^2)} = N(\underbrace{X}\bar{\beta}, \sigma^2)$

$\underline{\text{maximize } L(\beta)} : \beta^{MLE}$

$$L(\beta) = \prod_{i=1}^{N} f(x, y \mid \beta)$$

$\underbrace{P(\beta)}$ ← probability distribution on β

$$\tilde{L}(\beta) = L(\beta)$$

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Ridge Regression

$$P(\beta) = e^{-\delta^2 \|\beta\|_2^2}$$

$\|\cdot\|_2^2 \rightarrow$ L2 norm of vector

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Ridge Regression

$$\underline{P(\beta)} = e^{-\delta^2 \|\beta\|_2^2}$$

$\|\cdot\|_2^2 \rightarrow$ L2 norm of vector

$$\tilde{L}(\beta) = L(\beta)\, P(\beta)$$

$$= \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^N \exp\left(-\frac{1}{2}\|\bar{y} - X\bar{\beta}\|_2^2\right) \cdot \exp\left(-\delta^2 \|\beta\|_2^2\right)$$

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$$\log\left(\tilde{L}(\beta)\right) = -\frac{N}{2}\log\left(2\pi\sigma^2\right)$$

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$$\log(\tilde{L}(\beta)) = -\frac{N}{2}\log(2\pi\sigma^2) + \left(-\frac{1}{2}\|\bar{y} - X\bar{\beta}\|_2^2 - \delta^2\|\beta\|_2^2\right)$$

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Ridge Regression

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$$\underbrace{\log\left(\tilde{L}(\beta)\right)} = \underbrace{-\frac{N}{2}\log\left(2\pi\sigma^2\right)} + \underbrace{\left(-\frac{1}{2}\|\bar{y} - X\bar{\beta}\|_2^2 - \delta^2 \|\beta\|_2^2\right)}$$

minimize

$\rightarrow 0$

$\equiv$ minimize

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Ridge Regression

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$$\underbrace{\log\left(\tilde{L}(\beta)\right)} = \underbrace{-\frac{N}{2}\log(2\pi\sigma^2)}_{0} + \underbrace{\left(-\frac{1}{2}\|\bar{y} - X\bar{\beta}\|_2^2 - \delta^2 \|\beta\|_2^2\right)}$$

minimize

$$\equiv \text{minimize } \frac{1}{2}\|\bar{y} - X\bar{\beta}\|_2^2 + \delta^2 \|\beta\|_2^2$$

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$$\log(\tilde{L}(\beta)) = -\frac{N}{2}\log(2\pi\sigma^2) + \left(-\frac{1}{2}\|\bar{y} - X\bar{\beta}\|_2^2 - \delta^2\|\beta\|_2^2\right)$$

minimize

0

$$\beta_{reg} = \underset{\beta}{\text{minimize}} \; \frac{1}{2}\|\bar{y} - X\bar{\beta}\|_2^2 + \delta^2 \|\beta\|_2^2$$

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Ridge Regression

$$\frac{d}{d\beta} \log \tilde{L}(\beta) = 0$$

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Ridge Regression

$$\frac{d}{d\beta} \log \tilde{L}(\beta) = 0$$

$$\Rightarrow \quad \beta^{ridge} = \left(X^T X + \delta^2 I \right)^{-1} X^T \underline{y}$$

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Ridge Regression

$$\frac{d}{d\beta} \log \tilde{L}(\beta) = 0$$

$$\Rightarrow \quad \beta^{ridge} = \left(X^T X + \delta^2 \underbrace{I}_{\text{identity } r} \right)^{-1} X^T \underline{y}$$

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Ridge Regression

$$\frac{d}{d\beta} \log \tilde{L}(\beta) = 0$$

$$\Rightarrow \quad \beta^{ridge} = \left(X^T X + \delta^2 \underbrace{I}_{\text{identity matrix}} \right)^{-1} X^T \underline{y}$$

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LASSO Regression

$$P(\beta) = e^{-\delta^2 \|\beta\|_1}$$

$\|\cdot\|_1$ = L1 -norm of vector

$$\log \tilde{L}(\beta) = \log L(\beta) + \log P(\beta)$$

$$= -$$

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LASSO Regression

$$P(\beta) = e^{-\delta^2 \|\beta\|_1}$$

$\|\cdot\|_1$ = L1 -norm of vector

$$\log \tilde{L}(\beta) = \log L(\beta) + \log P(\beta)$$

$$= -\frac{N}{2}\log(2\pi\sigma^2) + \left(-\frac{1}{2}\|\bar{y} - X\bar{\beta}\|_2^2 - \delta^2\|\beta\|_1\right)$$

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$$= -\frac{N}{2}\log(2\pi\sigma^2) + \left(\underbrace{-\frac{1}{2}\|\bar{y} - X\bar{\beta}\|_2^2 - \delta^2\|\beta\|_1}\right)$$

$$\beta^{LASSO} = \min$$

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LASSO Regression

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$\|\cdot\|_1$ = L1 -norm of vector

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$$= -\frac{N}{2}\log(2\pi\sigma^2) + \underbrace{\left(-\frac{1}{2}\|\bar{y} - X\bar{\beta}\|_2^2 - \delta^2\|\beta\|_1\right)}$$

$$\beta^{LASSO} = \text{minimize} \underbrace{\left(\|\bar{y} - X\bar{\beta}\|_2^2 + \delta^2\|\beta\|_1\right)}$$

no closed form solution

gradient descent, SGD

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The Geometry of Regularization

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The fact that our loss function is now the **sum of two loss functions** gives us a new geometric interpretation.

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The Geometry of Regularization

The fact that our loss function is now the **sum of two loss functions** gives us a new geometric interpretation.

$$\text{loss function} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta^2 \|\beta\|.$$

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The fact that our loss function is now the **sum of two loss functions** gives us a new geometric interpretation.

$$\text{loss function} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta^2 \|\beta\|_{1/2}$$

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$$\text{loss function} = \underbrace{\|\bar{y} - X\bar{\beta}\|_2^2}_{L1} + \underbrace{\delta^2 \|\beta\|_{1/2}}_{L2}$$

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$$\text{loss function} = \underbrace{\|\bar{y} - X\bar{\beta}\|_2^2}_{\substack{L1 \\ \text{MLE}}} + \underbrace{\delta^2 \|\beta\|_{1/2}}_{\substack{L2 \\ \text{Reg}}}$$

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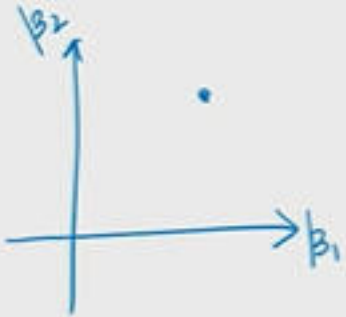

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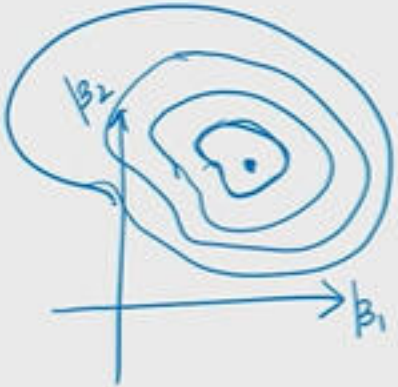

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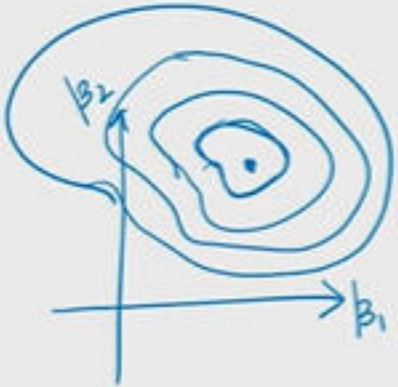

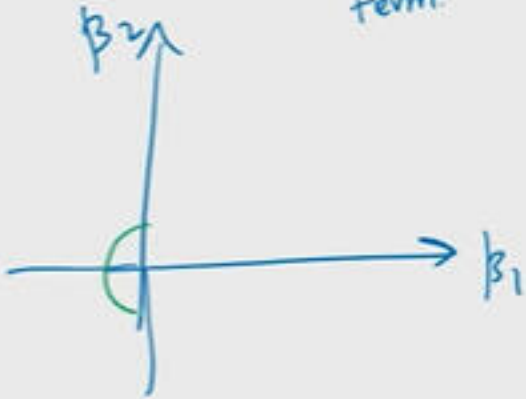

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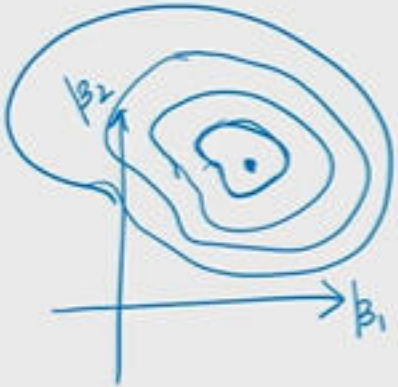

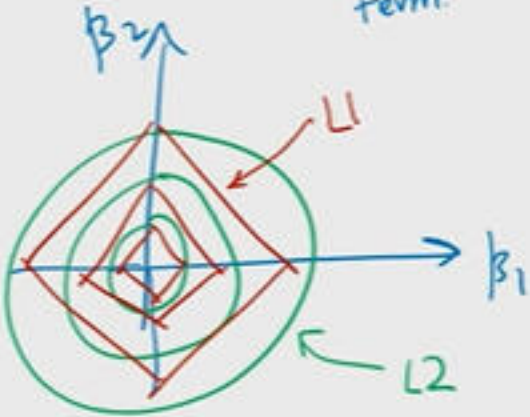

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The Geometry of Ridge Regularization

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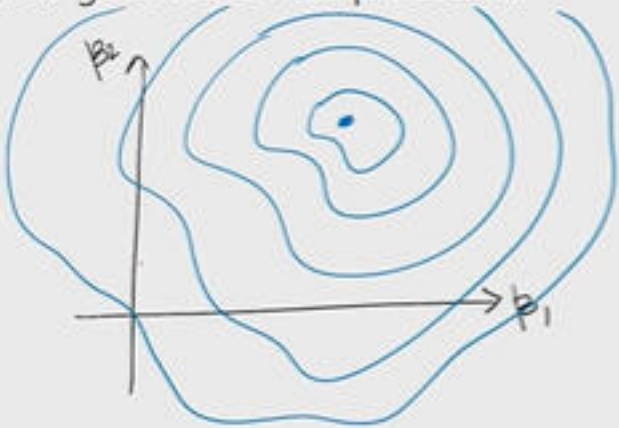

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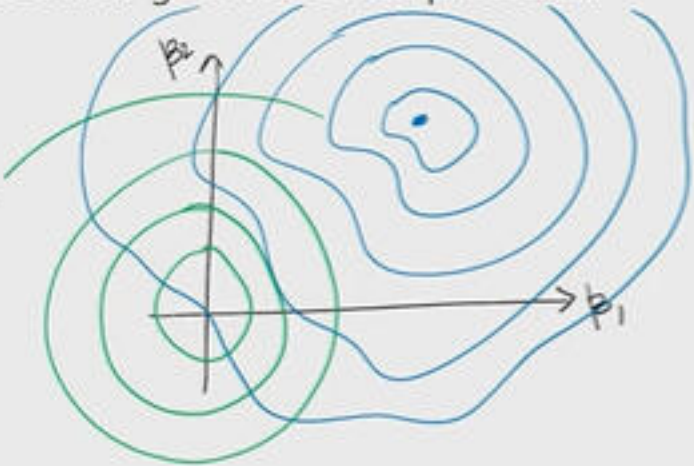

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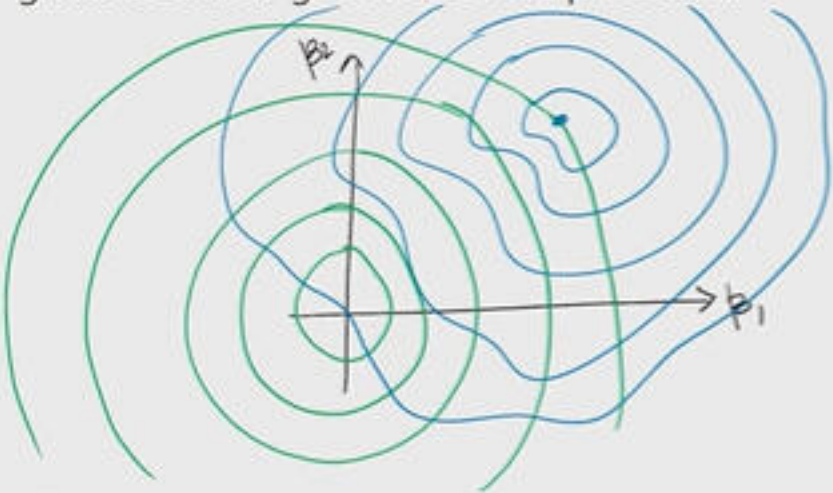

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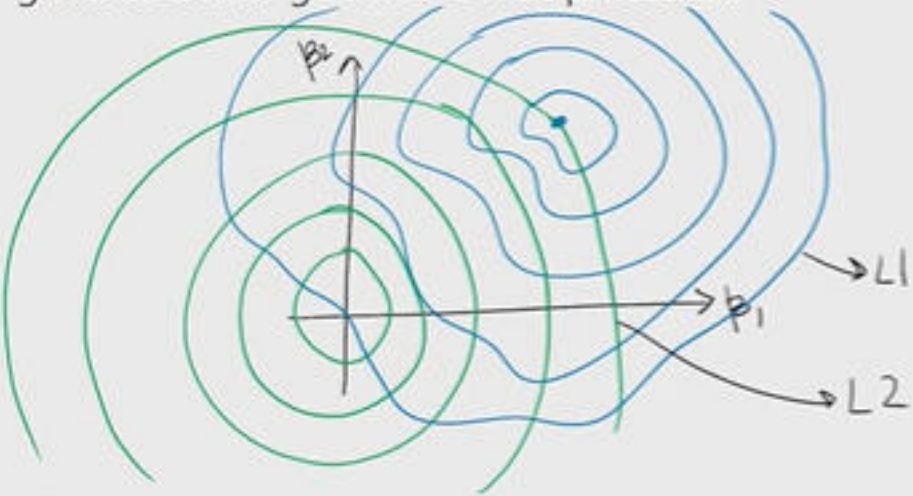

$$\frac{d\,\tilde{L}(\beta)}{d\beta} = 0$$

$$\frac{dL_1(\beta)}{d\beta} = -\frac{dL_2(\beta)}{d\beta}$$

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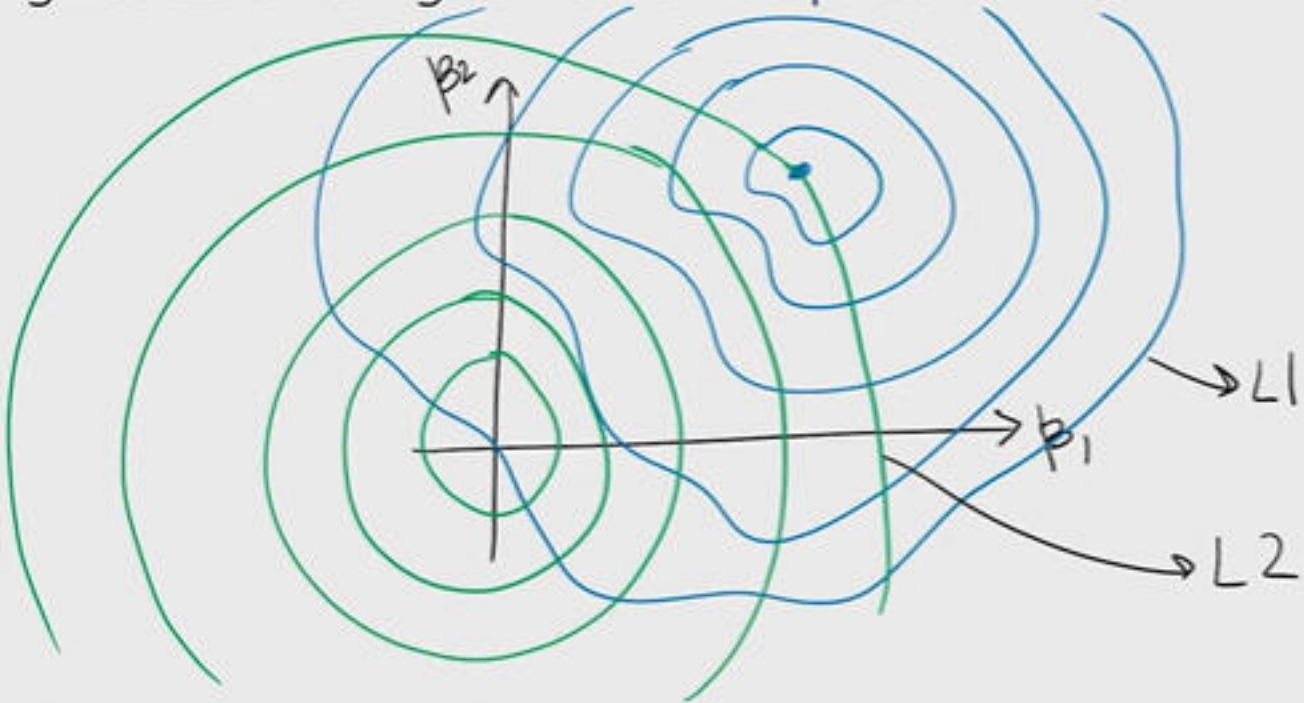

$$\frac{d\tilde{L}(\beta)}{d\beta} = 0$$

$$\underbrace{\frac{dL_1(\beta)}{d\beta}} = \underbrace{-\frac{\delta dL_2(\beta)}{d\beta}}$$

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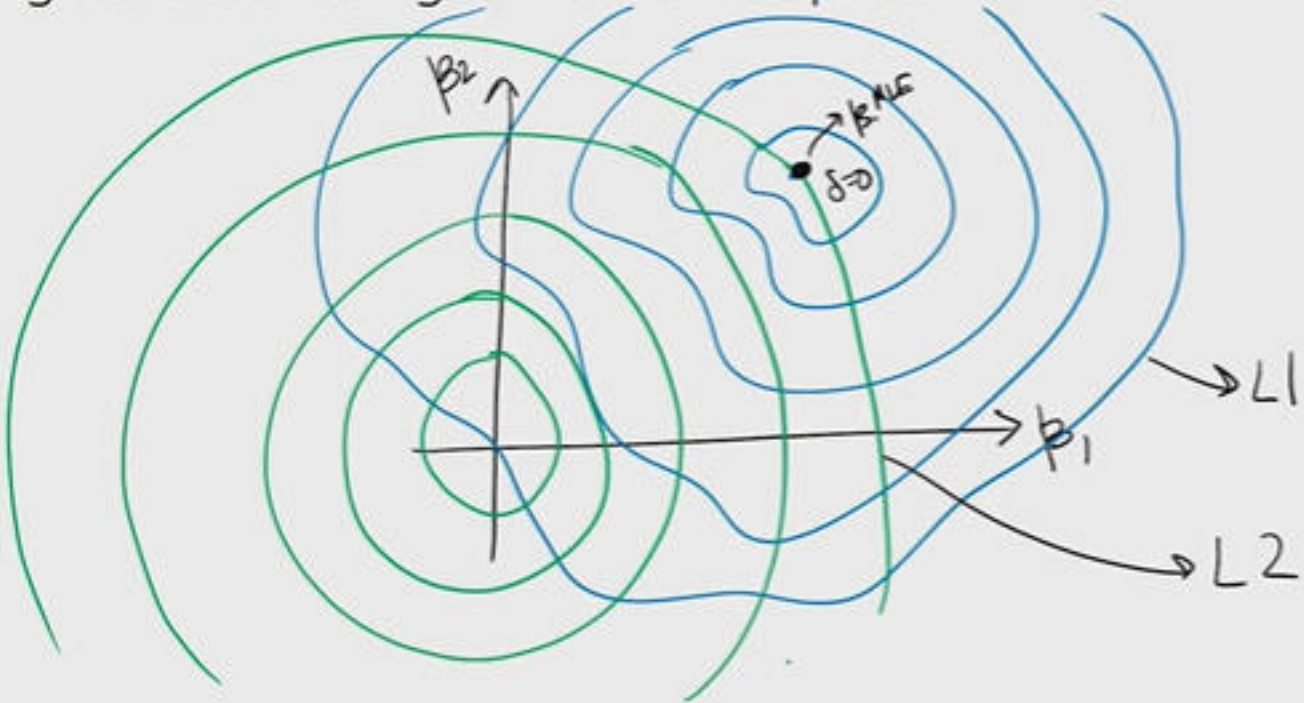

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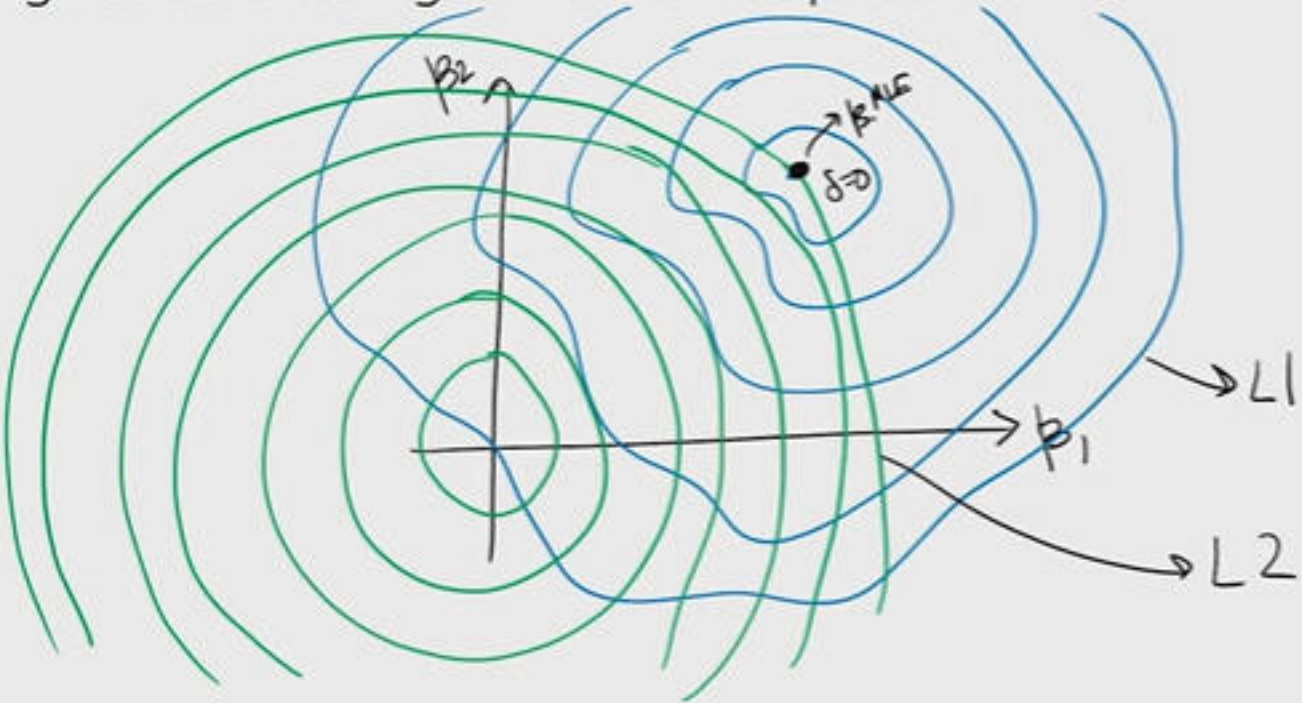

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The Geometry of Ridge Regularization

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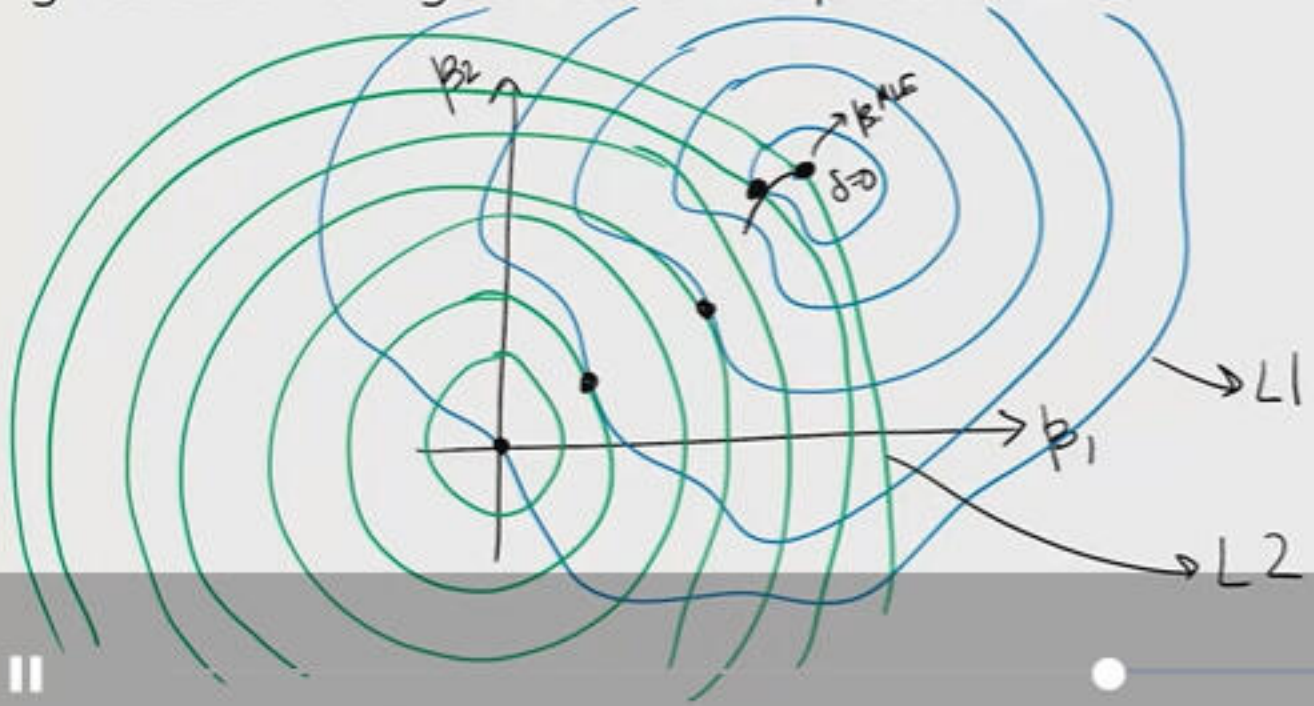

$$\frac{d\,\tilde{L}(\beta)}{d\beta} = 0$$

$$\underbrace{\frac{dL_1(\beta)}{d\beta}} = \underbrace{-\delta \frac{dL_2(\beta)}{d\beta}}$$

-5:04

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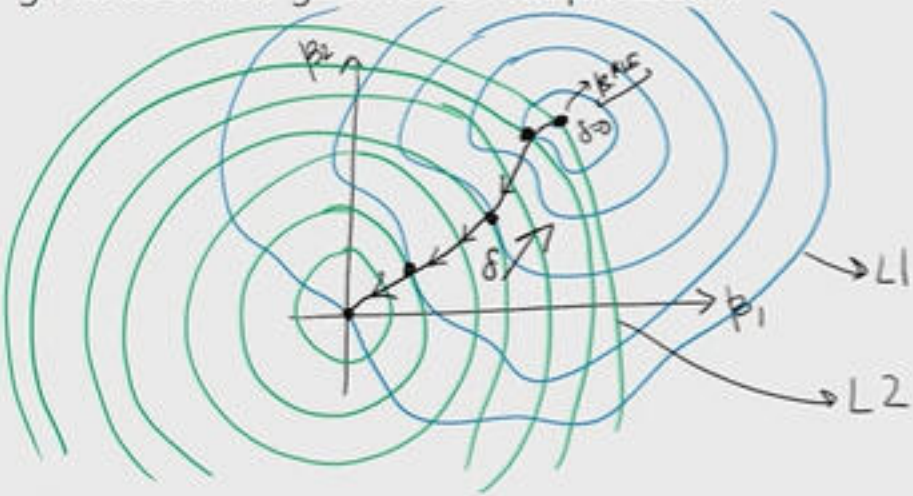

$$\frac{d\,\tilde{L}(\beta)}{d\beta} = 0$$

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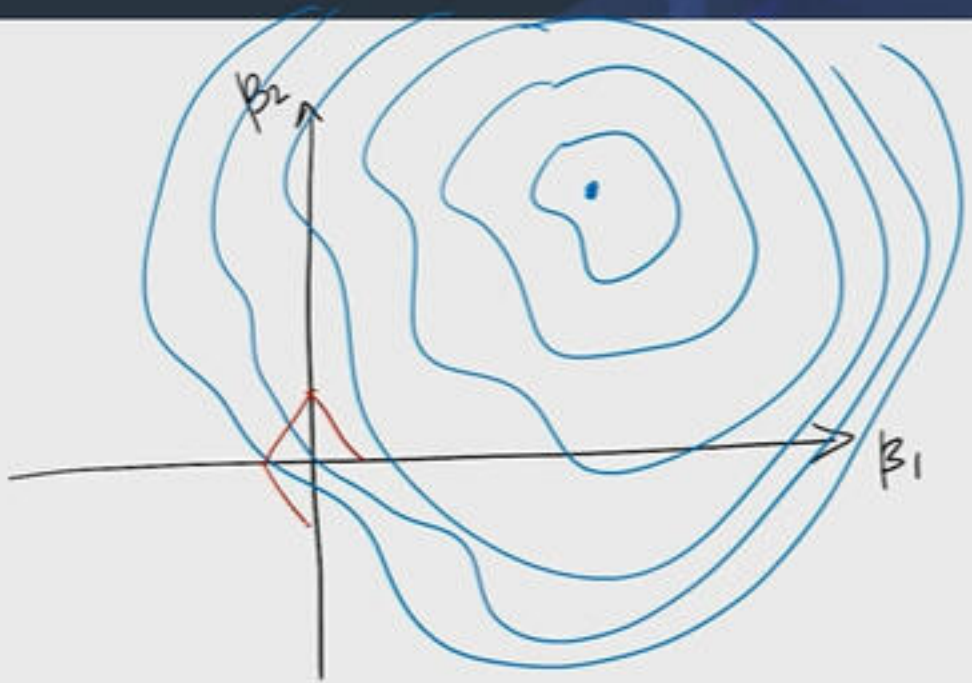
The Geometry of LASSO Regularization



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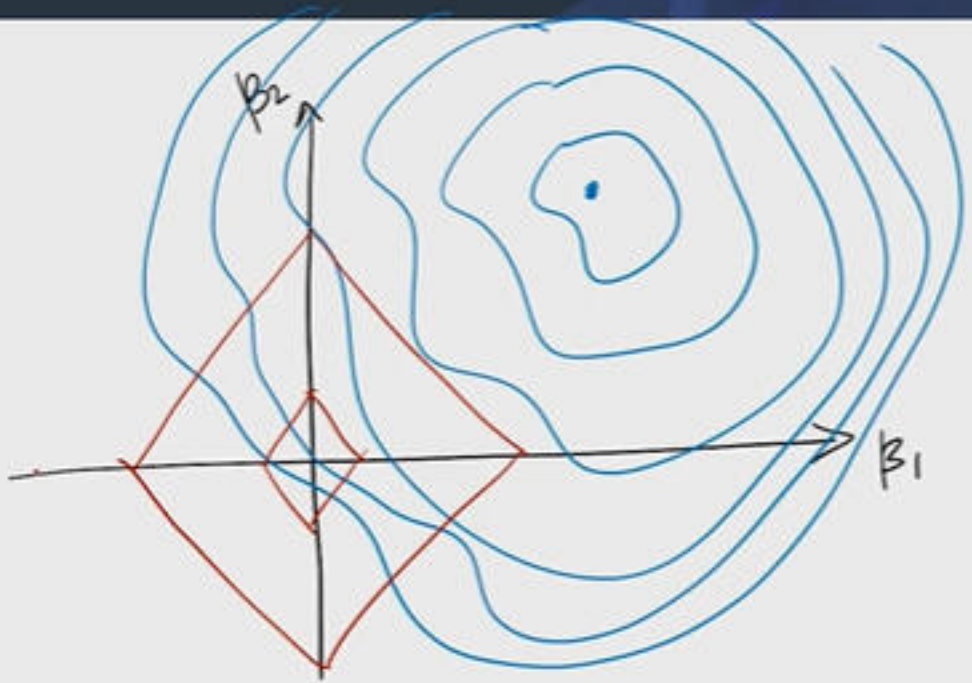
The Geometry of LASSO Regularization



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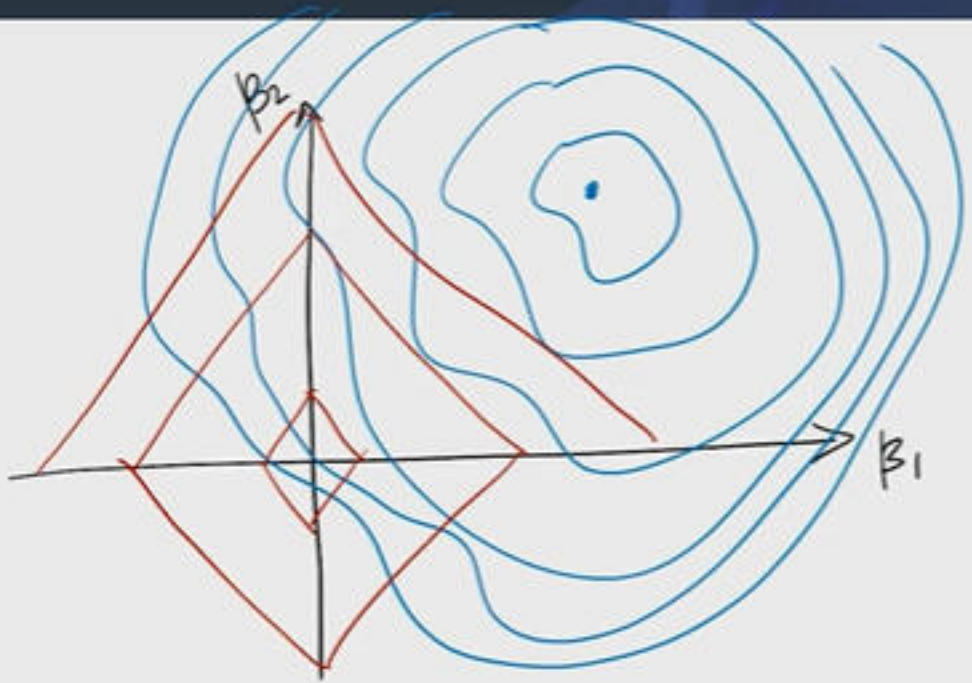

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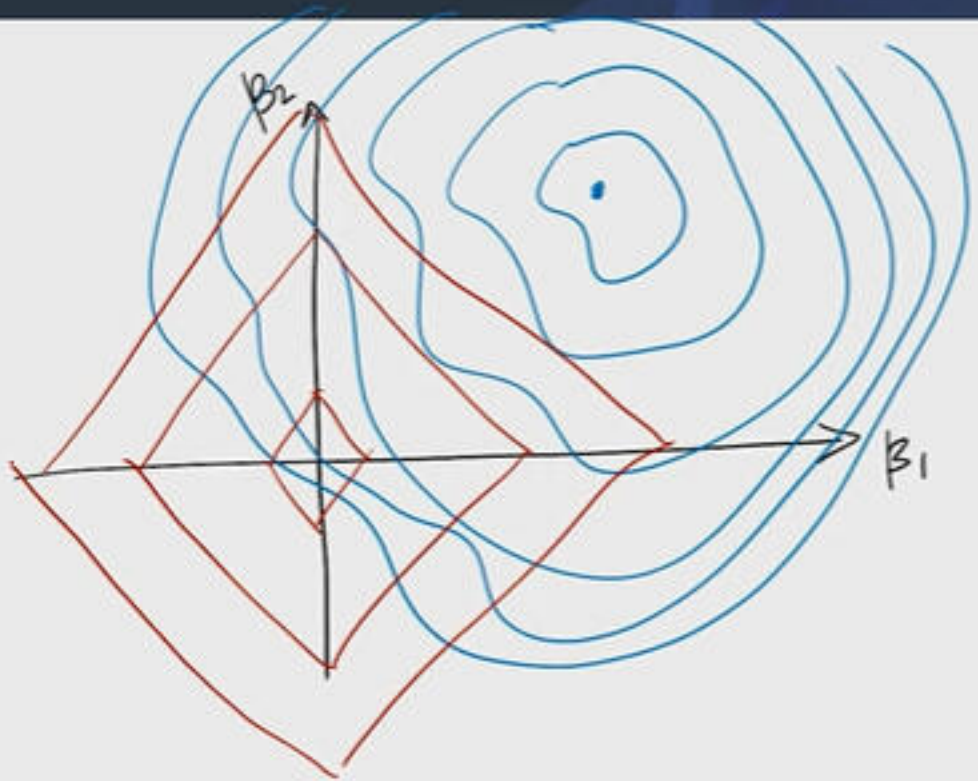
The Geometry of LASSO Regularization



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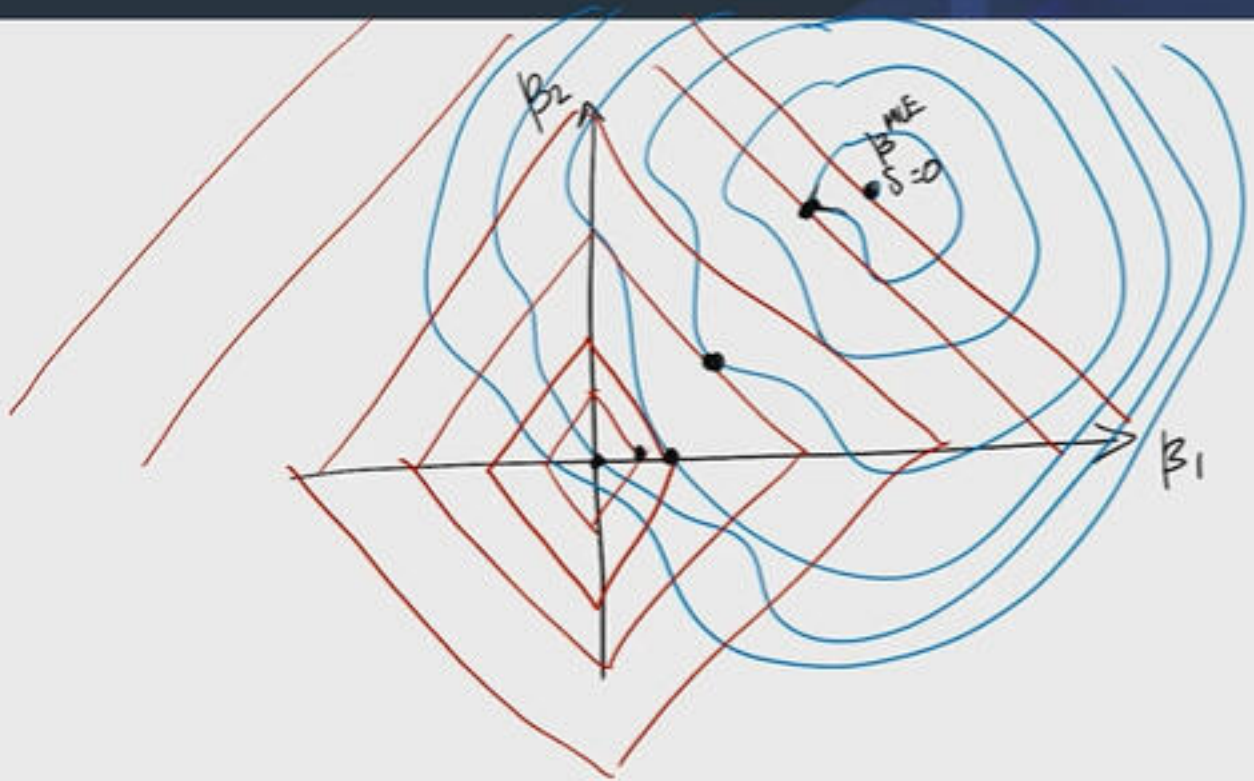
The Geometry of LASSO Regularization



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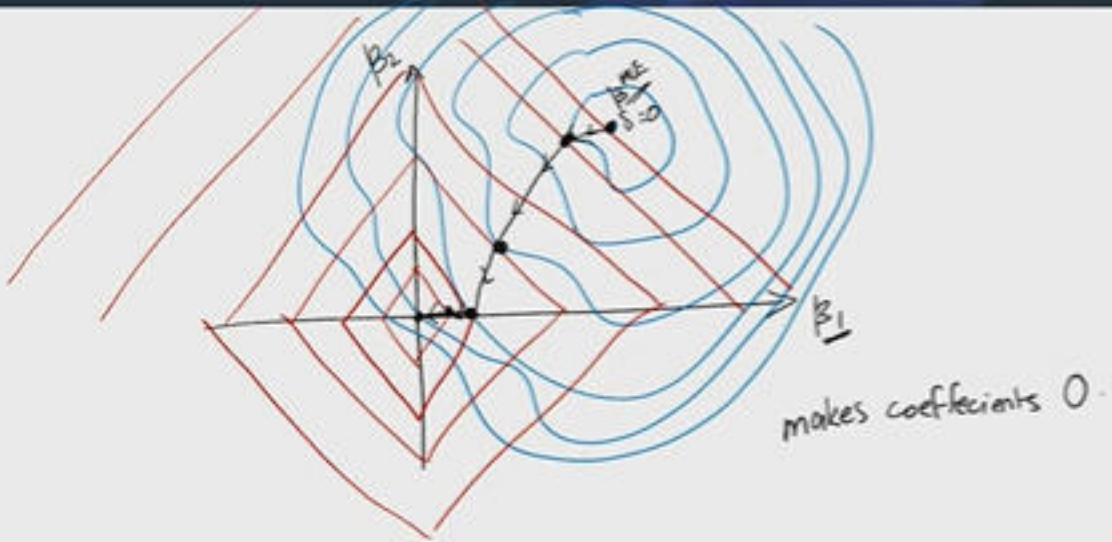
The Geometry of LASSO Regularization



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Elastic Net Regression

This is nothing more than a combination of the two previous techniques.

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Elastic Net Regression

This is nothing more than a combination of the two previous techniques.

$$L = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_1^2 \|\beta\|_1 + \delta_2^2 \|\beta\|_2^2$$

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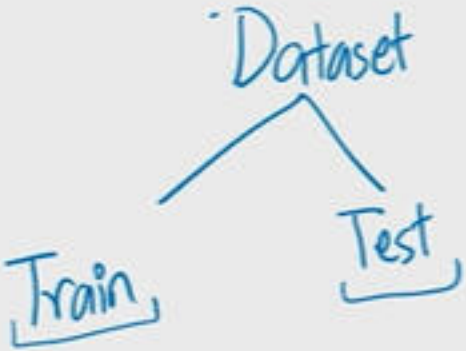
How do we pick δ ?



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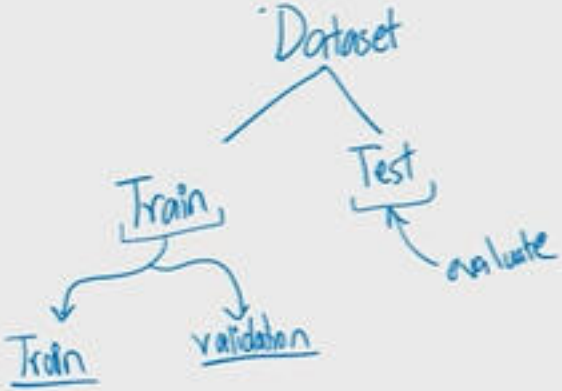
How do we pick δ ?



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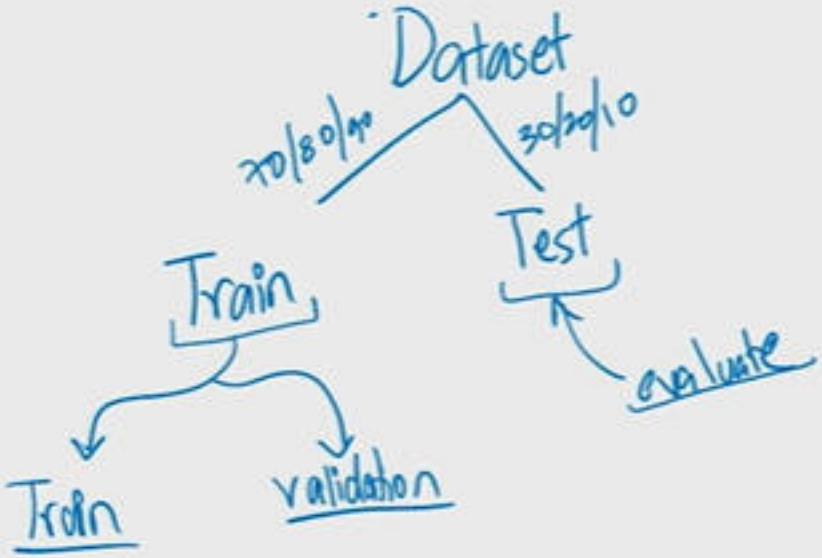

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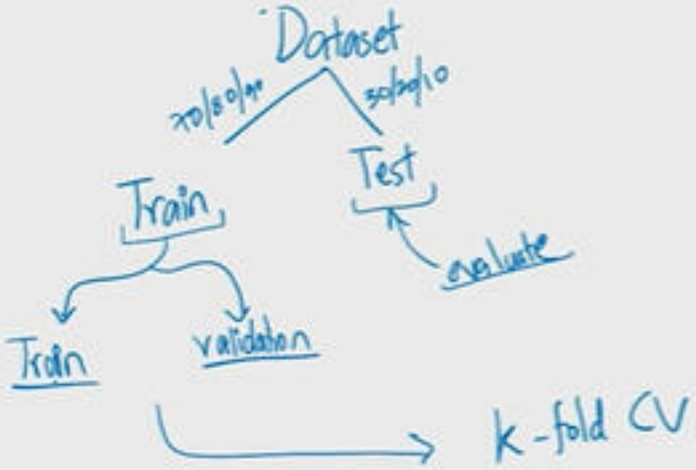

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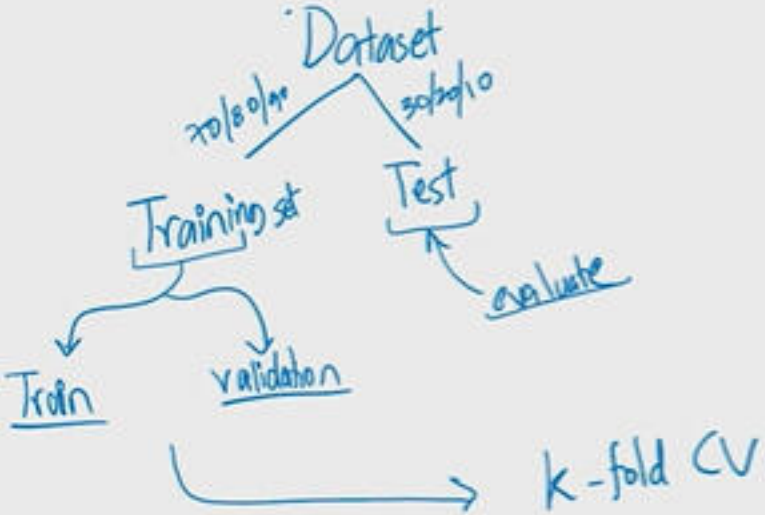

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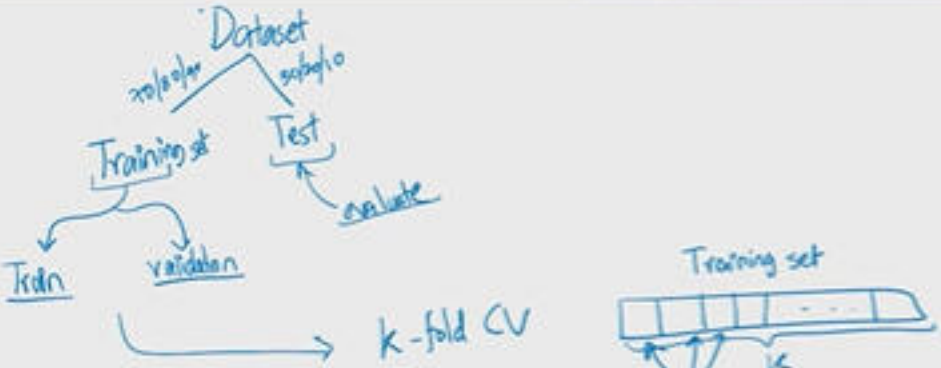
How do we pick δ ?



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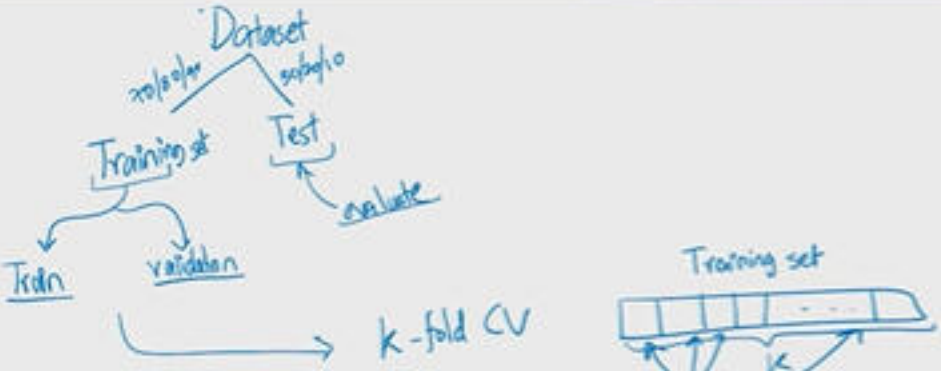

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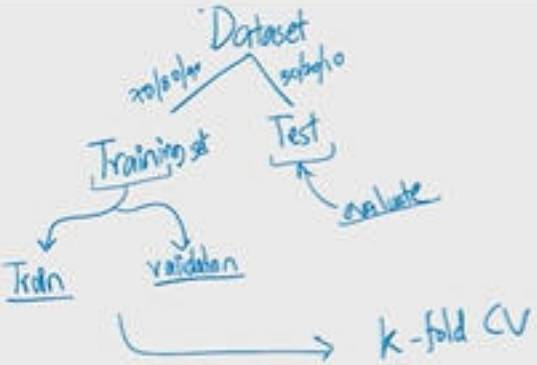

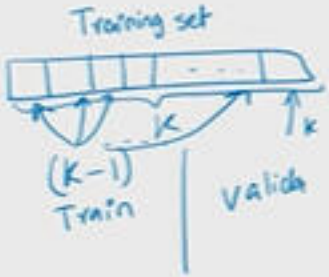

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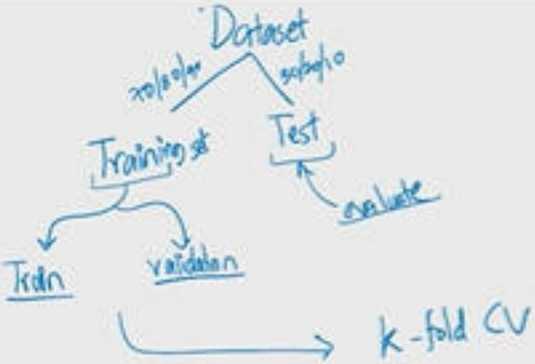
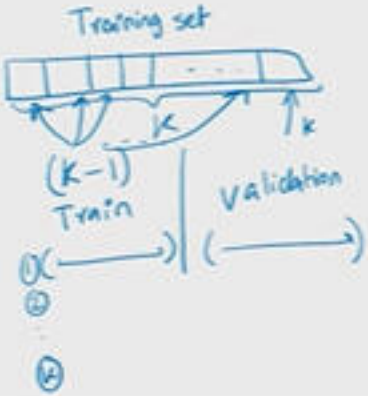
How do we pick δ ?





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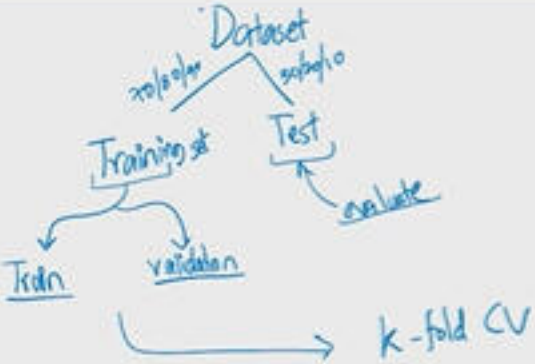

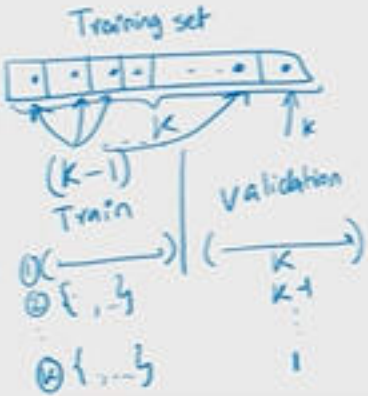

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Alternative Interpretation of Regularization

$$L = \|\bar{y} - X\bar{\beta}\|_2^2$$

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Alternative Interpretation of Regularization

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$$L = \|\bar{y} - X\bar{\beta}\|_2^2$$

unconstrained → overfitting

solution: penalize large values of "β".

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Alternative Interpretation of Regularization

Ridge regularization:

$$L = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta.$$

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Alternative Interpretation of Regularization

Ridge regularization:

$$L = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_2 \underbrace{\|\beta\|_2^2}_{\text{uniformly penalizes}}$$

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Alternative Interpretation of Regularization

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Ridge regularization:

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_2 \|\beta\|_2^2$$

uniformly penalizes

LASSO regularization,

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2$$

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Alternative Interpretation of Regularization

Ridge regularization:

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_2 \|\beta\|_2^2$$

uniformly penalizes

LASSO regularization,

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_1 \|\beta\|_1$$

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Ridge regularization:

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_2 \|\beta\|_2^2$$

uniformly penalizes

LASSO regularization:

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_1 \|\beta\|_1$$

unimportant coeff

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Alternative Interpretation of Regularization

Ridge regularization:

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_2 \|\beta\|_2^2$$

uniformly penalizes

LASSO regularization:

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_1 \|\beta\|_1$$

unimportant coeff $\rightarrow 0$

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Alternative Interpretation of Regularization

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Ridge regularization:

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_2 \|\beta\|_2^2$$

uniformly penalizes

LASSO regularization,

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_1 \|\beta\|_1$$

unimportant coeff $\to 0$

Elastic Net reg.:

$$\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta_1 \|\beta\|_1 + \delta_2 \|\beta\|_2^2$$

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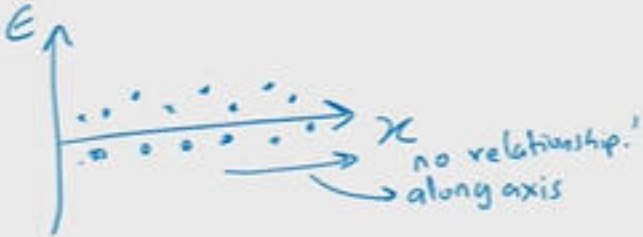
Non-Normality of Residuals?

Residual plot.



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Non-Normality of Residuals?

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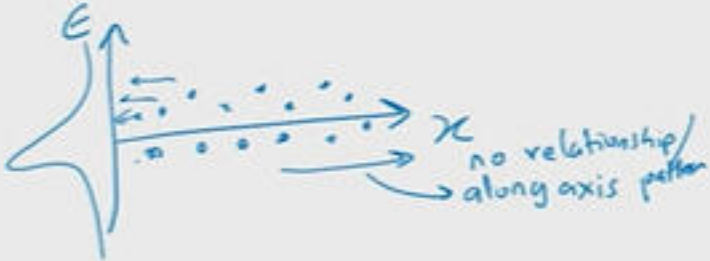
① Residual plot



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Non-Normality of Residuals?

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Identify ① Residual plot.

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Non-Normality of Residuals?

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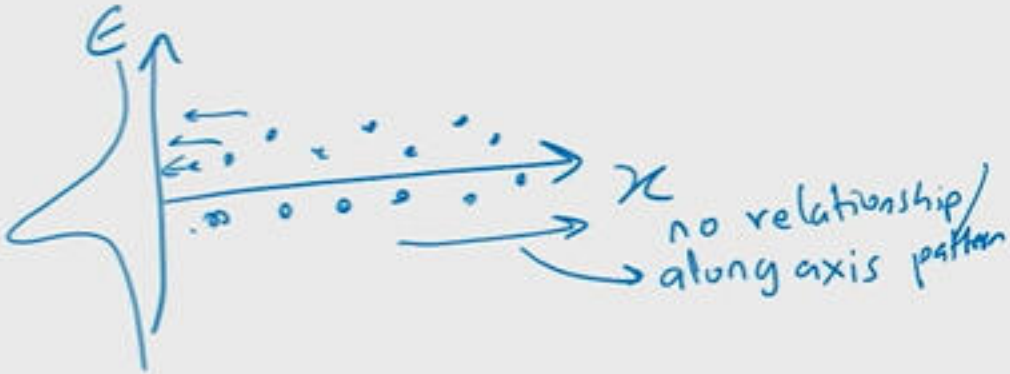
Identify

1. Residual plot.
2. Q-Q plot
3. Kolmogorov-Smirnov test.



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Non-Normality of Residuals?

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Identify
1. Residual plot
2. Q-Q plot
3. Kolmogorov-Smirnov test.

Model: 1. Poisson

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Non-Normality of Residuals?

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Identify
1. Residual plot
2. Q-Q plot
3. Kolmogorov-Smirnov test.

Model:
1. Poisson
2. Exponential

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$X^T X$ Not Invertible

$$\beta^* = (X^T X)^{-1} X^T \underline{y}$$

$$\hat{y} = X\bar{\beta}$$

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$X^T X$ Not Invertible

$$\hat{y} = X\bar{\beta}$$

$$\beta^* = \underbrace{(X^T X)}^{-1} X^T \underline{y}$$

$$\beta^{\text{ridge}} = (\underbrace{X^T X}_{\text{p.s.d}} + \lambda^2 \underbrace{I}_{\text{identity matrix}})^{-1} X^T \underline{y}$$

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$X^T X$ Not Invertible

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$$\hat{\bar{y}} = X\bar{\beta}$$

$$\beta^* = \underbrace{(X^T X)}^{-1} X^T \underline{y}$$

$$\beta^{ridge} = \underbrace{\left(\underbrace{X^T X}_{p.s.d} + \lambda^2 \underbrace{I}_{pd}\right)}_{pd}^{-1} X^T \underline{y}$$

identity matrix

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$X^T X$ Not Invertible

$$\hat{\underline{y}} = X\bar{\beta}$$

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identity matrix

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Classification and Logistic Regularization

The OLS model is the best approximation model to predict data structures. However, you can't use it directly because the end model format doesn't fit the classification approach. In this course, we will explore a classification model that provides a finite number of discrete labels.

The following topics will be covered:

- The math behind logistic regression
- Visualizing logistic regression
- Logistic regression loss function and minimizing log likelihood function
- Batch/Full logistic regression
- Gradient descent for OLS

The following topics will be covered:

- The math behind logistic regression
- Visualizing logistic regression
- Logistic regression loss function and minimizing log likelihood function
- Batch/Full logistic regression
- Gradient descent for OLS
- Gradient descent for logistic regression
- Comparing OLS and logistic regression
- Multi-class logistic regression using Softmax function

Logistic Regression

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- Ordinary Least Squares (OLS)
- Logistic Regression
- The Setup
- The Issue
- Definitions
  - Link function
  - Logistic function
- Note on Choice of Link
- Visualizing Logistic Regression

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Logistic Regression Loss

- Our Goal
- The Full Log-Likelihood
- A Note on Minimization

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(Batch/Full) Gradient Descent

- The Gradient
- Algorithm

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Gradient Descent for Logistic Regression

- Numerical Minimization of Logistic Loss
- Hard Term
- Hard Term 2
- All Terms

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Summary of Calculations

- Written Out Nicely
- A Note on Normalization
- The Algorithm

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Comparison with OLS

- The Two Update Steps
- Regularization

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Beyond Two Types

- The Softmax
- Comparison with Logistic Regression in the Case of Two Types

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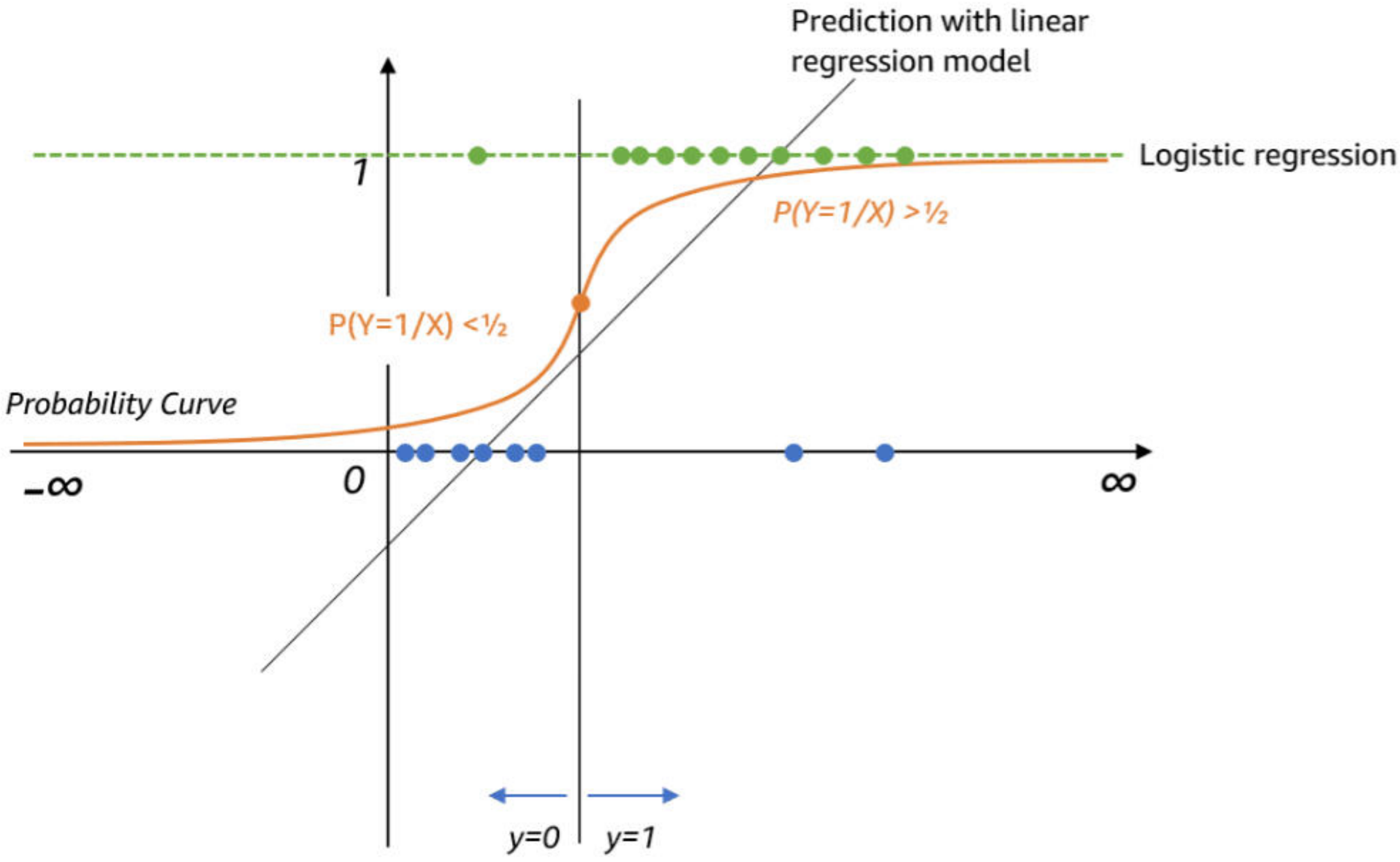
Prediction with linear regression model
Logistic regression
1
P(Y=1/X) >½
P(Y=1/X) <½
Probability Curve
-∞
0
∞
y=0
y=1

Topics

- Ordinary Least Squares (OLS)
- The Issue
- Logistic Regression

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Topics

- Ordinary Least Squares (OLS)
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- The Setup

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Topics

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OLS

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This is regression.

Predicts continuous and potentially unbounded labels based on given features.

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OLS

aws training and certification

This is regression.

Predicts continuous and potentially unbounded labels based on given features.

$$\hat{\bar{y}} = \underbrace{X}_{\text{data matrix}}\bar{\beta}$$

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The Issue

unbounded output $\not\Rightarrow$ classification.

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Logistic Regression

This is classification.

Predicts discrete labels based on given features.

The Setup

$$y = \begin{matrix} 0 \\ 1 \end{matrix}$$

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The Setup

$x,$ $\quad y = \begin{matrix} 0 \\ 1 \end{matrix} \quad \left.\begin{matrix} 1-p \\ p \end{matrix}\right\}$ probability

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The Setup

$x,$ $\quad y = \begin{matrix} 0 & 1-p \\ 1 & p \end{matrix} \Big\}$ probability

estim $\quad \boxed{P(y=1 \mid X)}$

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Definitions

Link function

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Definitions

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Link function

relates mean of distribution to output of linear model

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Definitions

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Link function

relates mean of distribution to output of linear model.

- unbounded ⇒ bounded
- continuous ⇒ discrete interpretation

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Definitions

Logistic function

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Definitions

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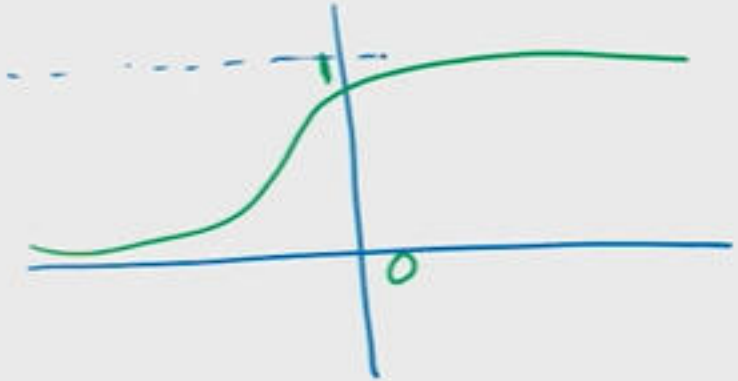
Logistic function



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Definitions

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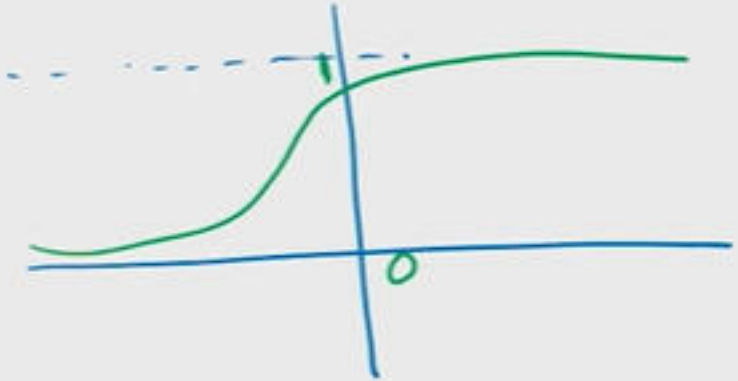
Logistic function



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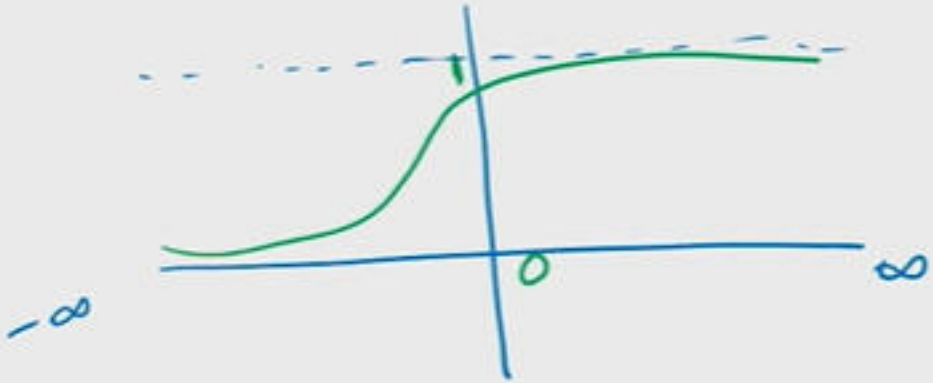
Definitions

Logistic function



$$f : (-\infty, \infty) \to (0, 1)$$

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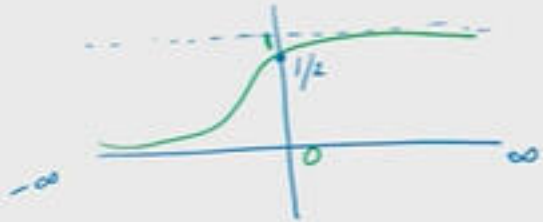
Definitions

aws training and certification

Logistic function



$f(0) = 1/2$

$f(-\infty) = 0$

$f(\infty) = 1$

① $f : (-\infty, \infty) \to (0, 1)$

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-6:44

Definitions

Logistic function

$f(0) = 1/2$

$f(-\infty) = 0$

$f(\infty) = 1$

① $f : (-\infty, \infty) \to (0,1)$

$\mathbb{P}(Y=1 \mid X)$

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Note on Choice of Link

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① bounded [0,1]

②

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Note on Choice of Link

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① bounded $[0,1]$

② domain $(-\infty, \infty)$

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Note on Choice of Link

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1. bounded $[0,1]$
2. domain $(-\infty, \infty)$
3. differentiable everywhere.
4. increasing function.

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Visualizing Logistic Regression

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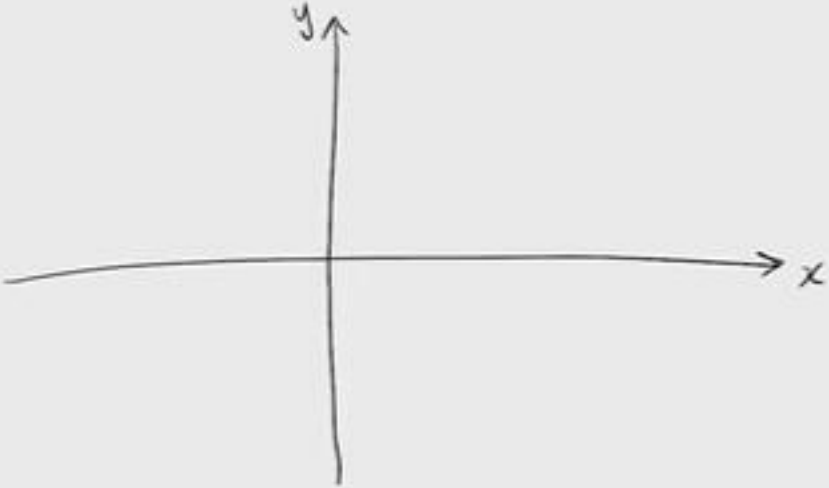

$y \in \{0, 1\}$

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Visualizing Logistic Regression

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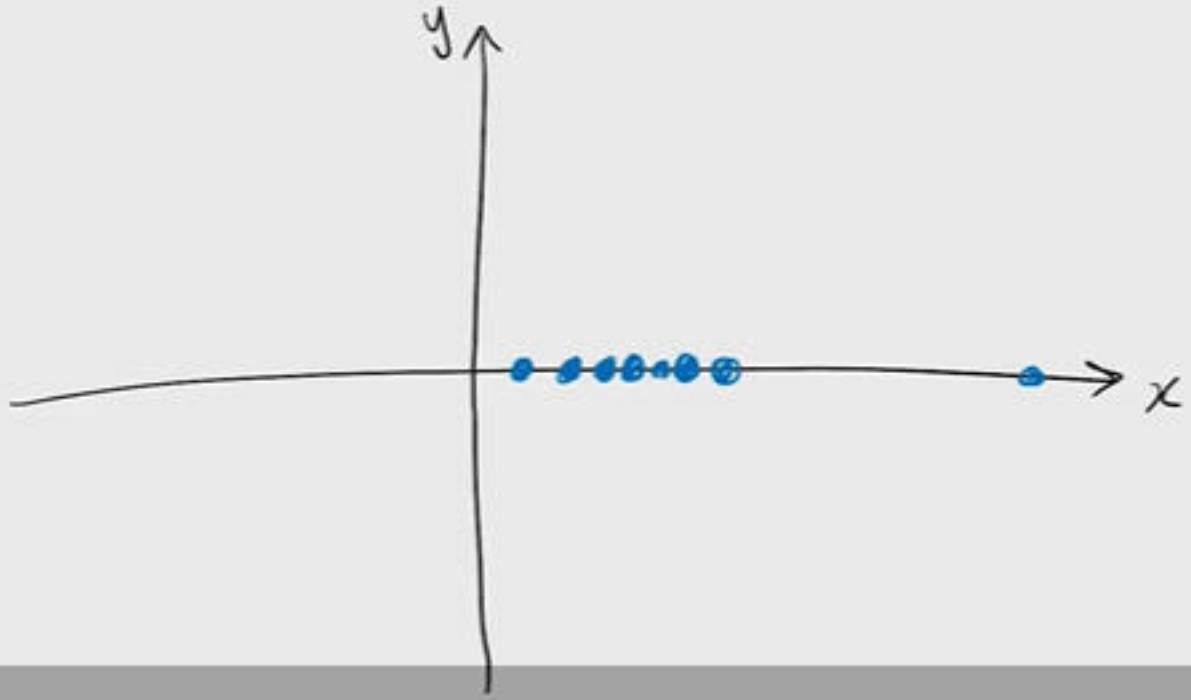

$y \in \{0, 1\}$

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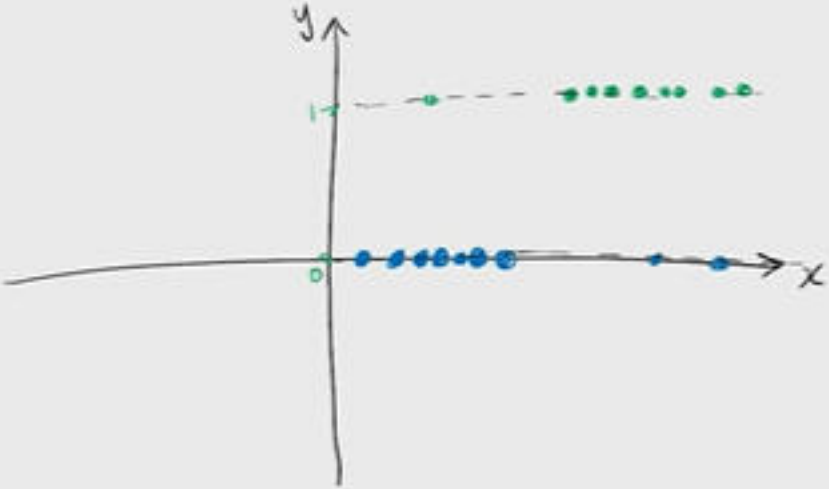
Visualizing Logistic Regression



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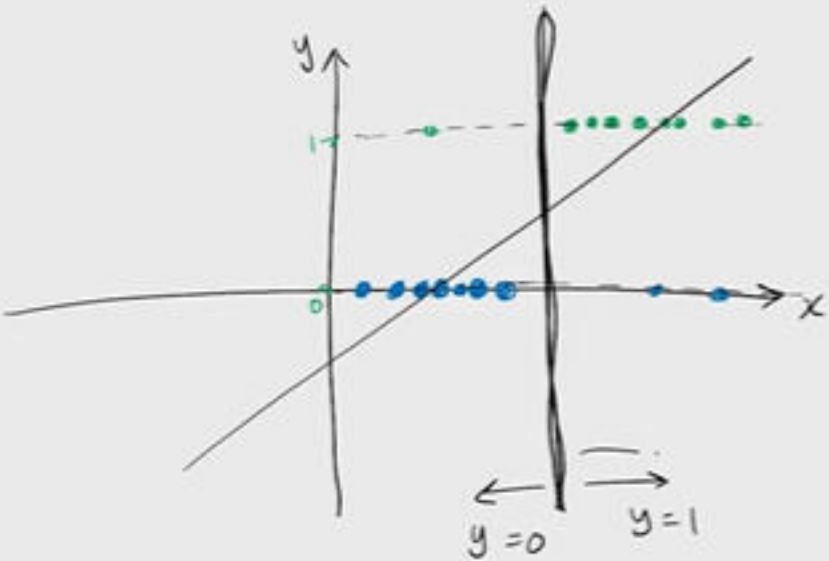
Visualizing Logistic Regression



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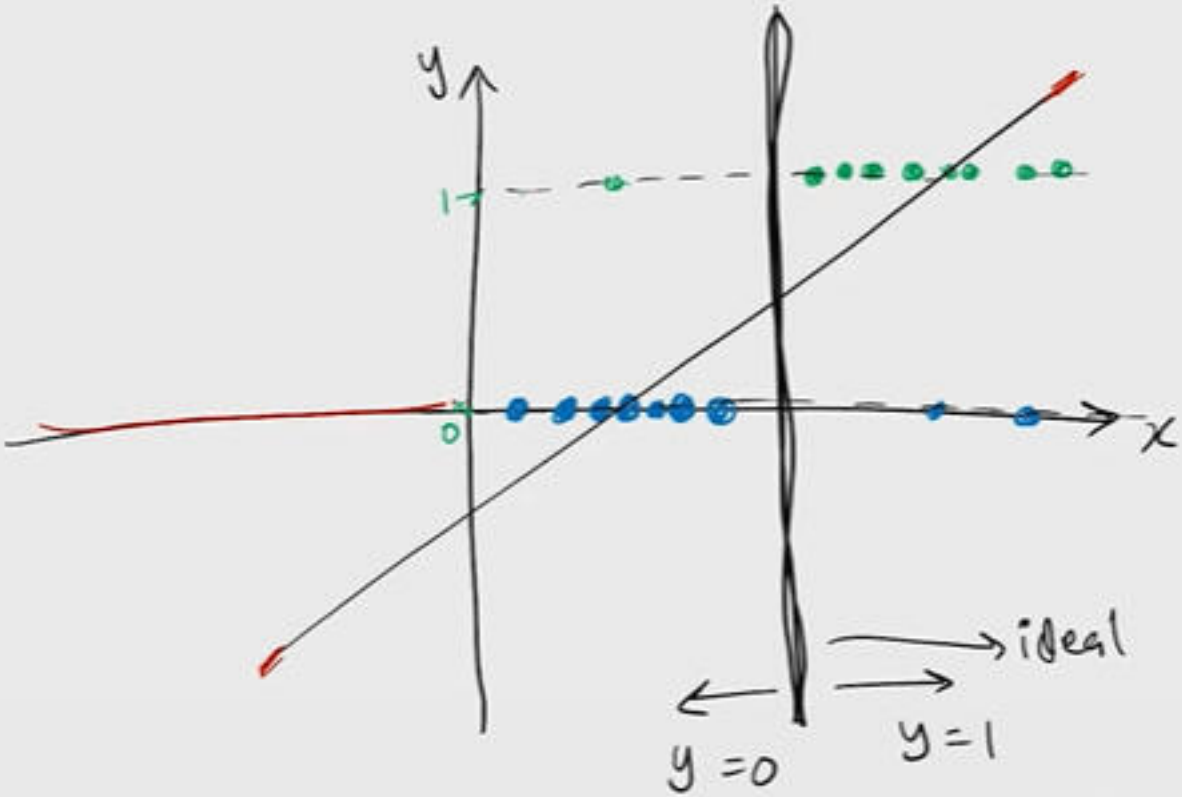
Visualizing Logistic Regression



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Visualizing Logistic Regression

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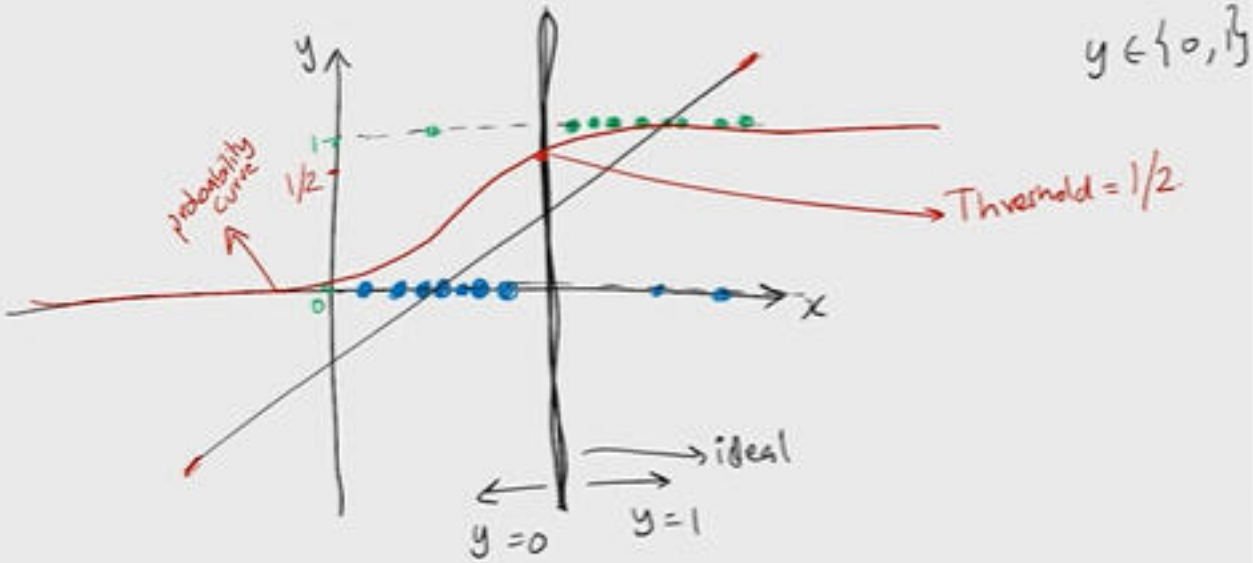

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Logistic Regression Loss

In this video we define the loss function for logistic regression and find its full log-likelihood estimation that we can minimize. However, unlike the OLS model, the logistic loss function doesn't have explicit solutions, so we'll need to minimize it numerically. Take a moment to explore before watching the video.

To find the logistic regression loss function:

1. Start with the logistic regression problem.
2. Find the full log likelihood.
3. Minimize -log(L).

Our Goal

$$\underbrace{P(y=1|X)}_{\text{probability to be estimated}}$$

$$\phi(x) = \frac{1}{1+e^{-x}}$$

$$\bar{y} = X\bar{\beta}$$

$$\boxed{\bar{y} = \Phi(X\bar{\beta})}$$

$$\Phi = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$

$$y_i = \phi(\bar{x}_i \cdot \bar{\beta})$$

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Our Goal

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MLE: $\mathcal{L} = \prod_{i=1}^{N} P(Y=y_i | \bar{x}_i$

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Our Goal

$Y = \begin{cases} 0 \\ 1 \end{cases}$ $\quad \underbrace{P(y=1|X)}_{\text{probability to be estimated}}$

Bernoulli $\rightarrow p$

$$\phi(x) = \frac{1}{1+e^{-x}}$$

$$\underbrace{\bar{y} = X\bar{\beta}}$$

$$\boxed{\bar{y} = \Phi(X\bar{\beta})}$$

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$$y_i = \phi(\bar{x}_i \cdot \bar{\beta})$$

MLE;

$$\mathcal{L} = \prod_{i=1}^{N} P(Y=y_i|\bar{x}_i) = \prod_{i=1}^{N} (p)^{y_i}(1-p)^{1-y_i}$$

$\leftarrow$ independent (joint $\rightarrow$ product)

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Our Goal

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$Y = \begin{cases} 0 \\ 1 \end{cases}$ $\quad \underbrace{P(y=1|X)}_{\text{probability to be estimated}}$

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MLE ;

$$L = \prod_{i=1}^{N} P(Y=y_i \mid \bar{x}_i) = \prod_{i=1}^{N} (p)^{y_i}(1-p)^{1-y_i}$$

$\leftarrow$ independent (joint $\rightarrow$ product)

log-likelihood, $\log(L) =$

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-3:29

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$=$

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$\hookrightarrow P(y_i | \bar{x}_i)$

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neg. log likelihood : $\boxed{-\log(\mathcal{L})}$

-1:14

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Our Goal

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minimize

neg. log likelihood : $\boxed{-\log(\mathcal{L})}$

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The Full Log-Likelihood

$$\mathcal{L}(\vec{\beta}) = -\sum_i \left[y_i \log(\phi(\vec{x_i} \cdot \vec{\beta})) + (1 - y_i)\log(1 - \phi(\vec{x_i} \cdot \vec{\beta}))\right]$$

minimize
in
Logistic

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A Note on Minimization

This does not have an explicit solution,
so we need to
minimize numerically

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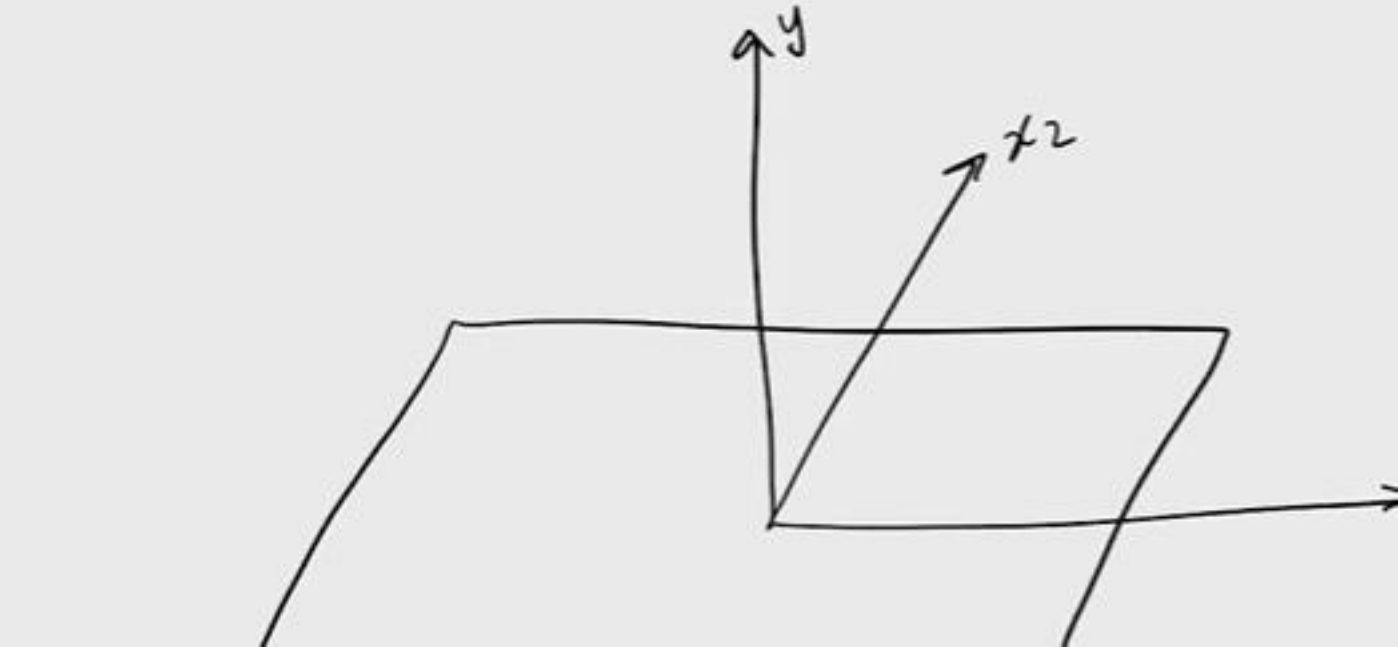
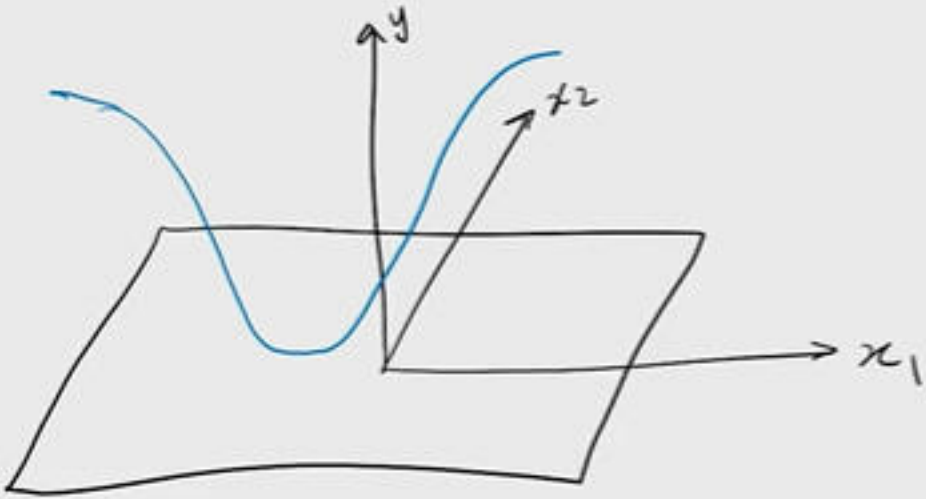
The Gradient



The Gradient



$y = f(x_1, x_2)$

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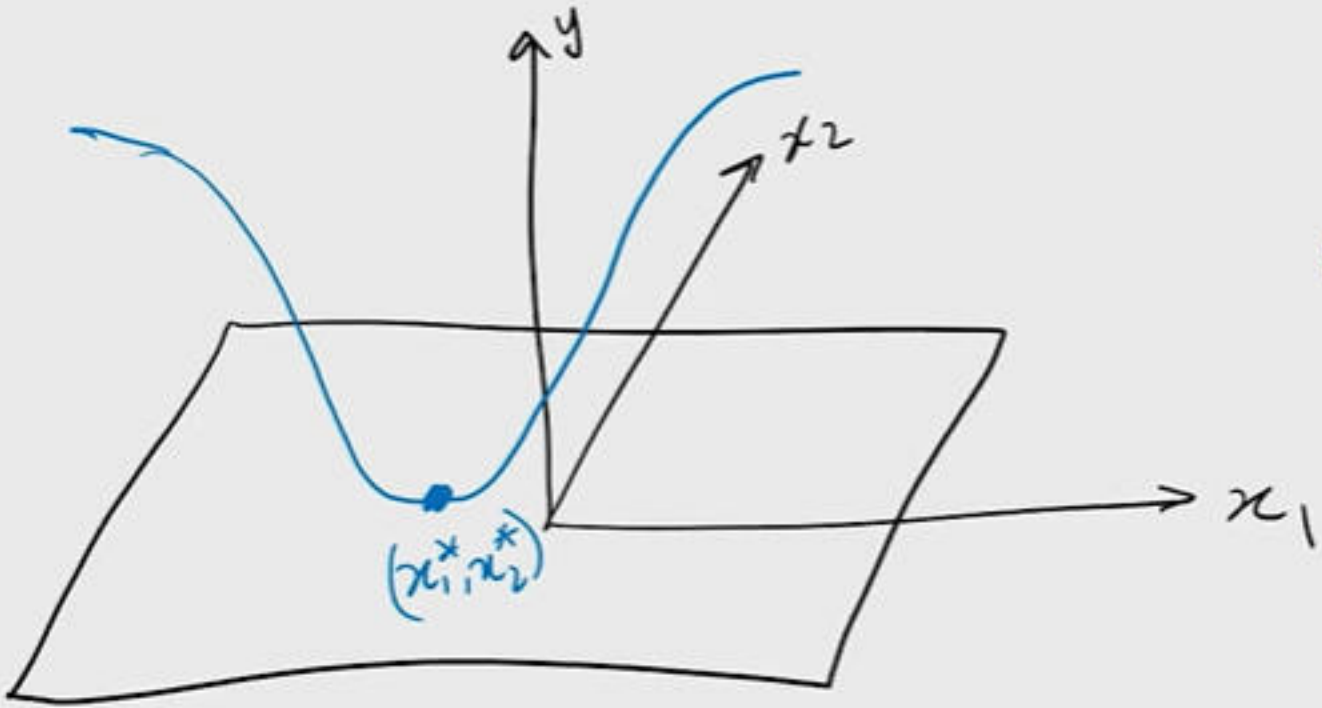
The Gradient



$y = f(x_1, x_2)$

$x_1^*, x_2^* = \arg\min$

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The Gradient

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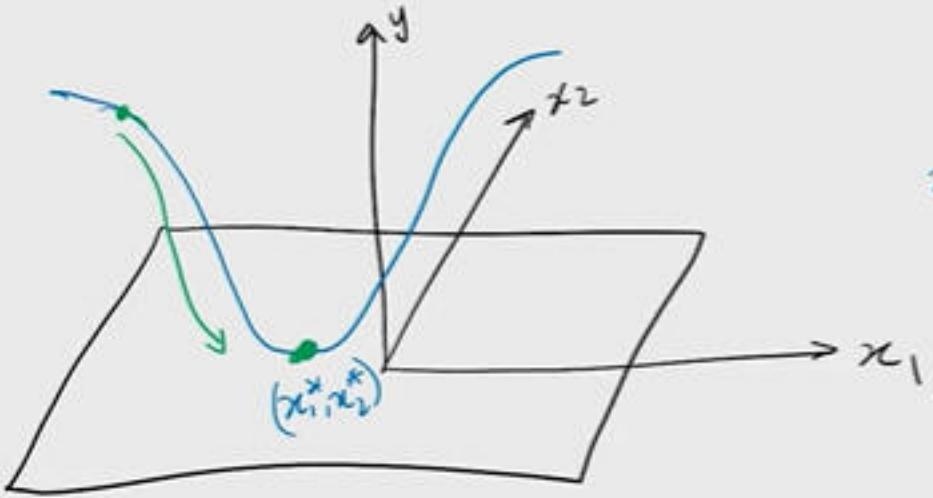

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$x_1^*, x_2^* = \arg\min_{x_1, x_2} f(x_1, x_2)$

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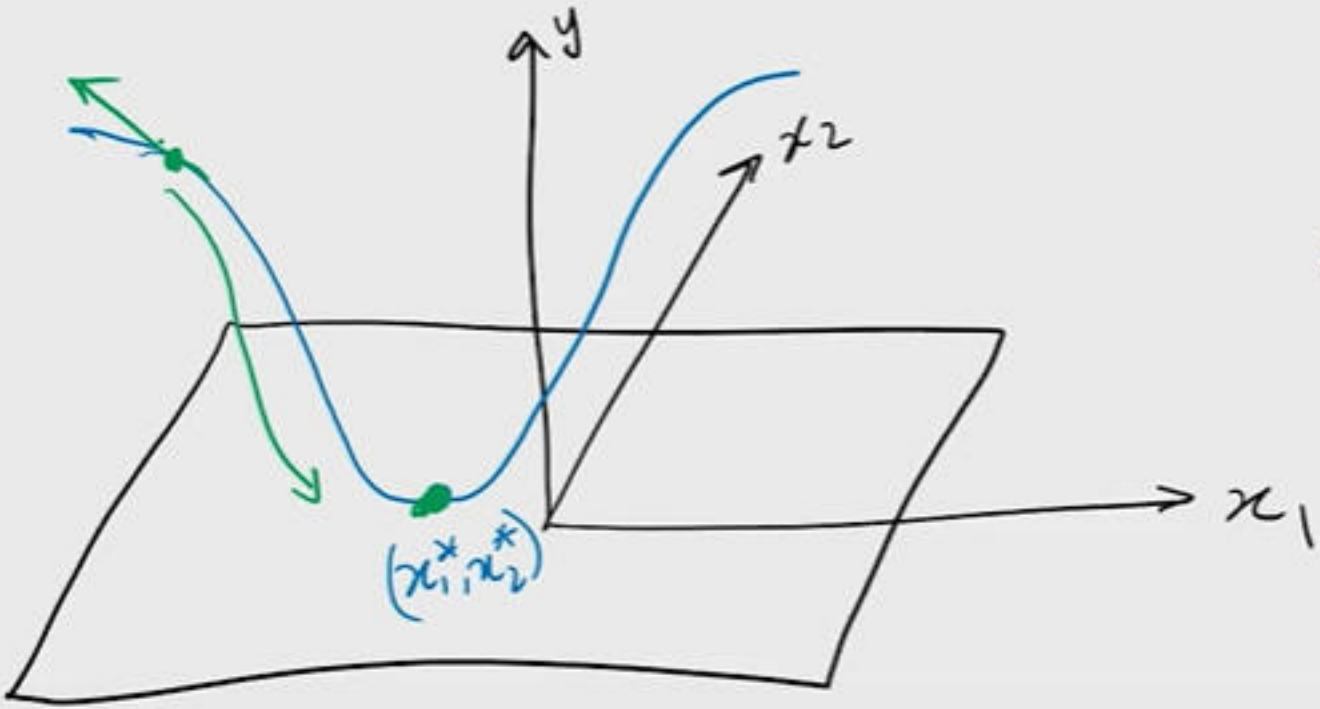
The Gradient



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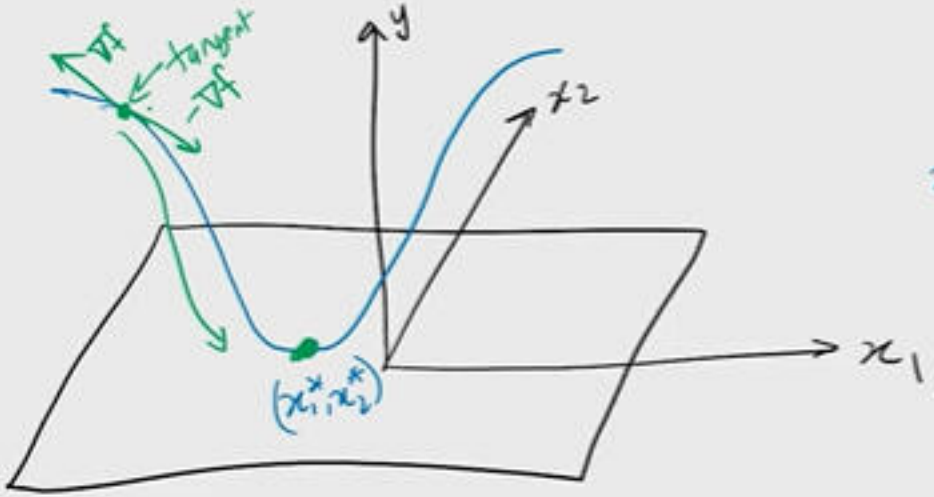

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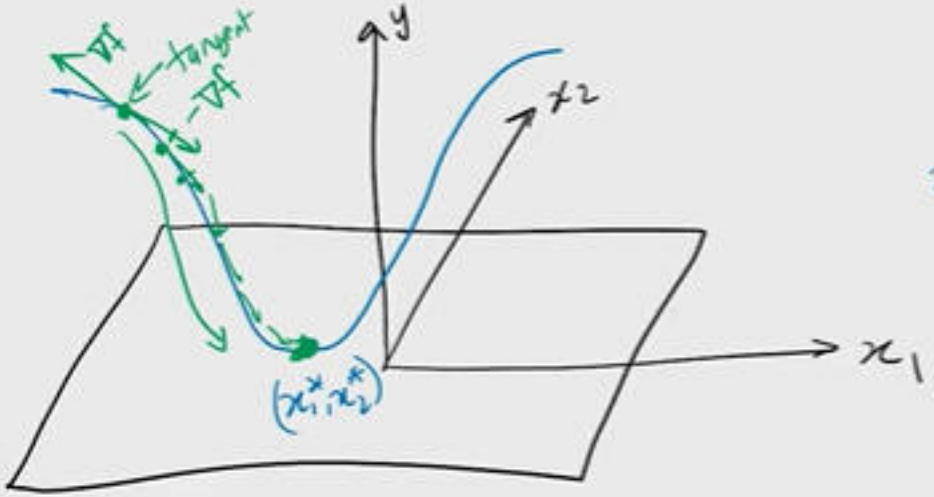

$y = f(x_1, x_2)$

$x_1^*, x_2^* = \arg\min_{x_1, x_2} f(x_1, x_2)$

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Algorithm

① Random choice of $\bar{x}$

② Compute gradient of f at $\bar{x}$ $\nabla f(\bar{x})$

③ Step in the direction of the negative of the gradient.

x:

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Algorithm

1. Random choice of $\bar{x}$
2. Compute gradient of f at $\bar{x}$ $\nabla f(\bar{x})$
3. Step in the direction of the negative of the gradient.

$$\bar{x} \leftarrow \bar{x} - \underbrace{\eta}_{\text{step size}} \nabla f(\bar{x})$$

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Algorithm

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① Random choice of $\bar{x}$

② Compute gradient of f at $\bar{x}$ $\nabla f(\bar{x})$

③ Step in the direction of the negative of the gradient.

$$\bar{x} \leftarrow \bar{x} - \eta \nabla f(\bar{x})$$

η → step size → how fast do you want to minimize?

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Numerical Minimization of OLS

We work with the **mean log-likelihood**.

!

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Numerical Minimization of OLS

We work with the **mean log-likelihood**.

$$L = -\frac{1}{N} \|\bar{y} - X\bar{\beta}\|_2^2$$

N - observations.

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Numerical Minimization of OLS

We work with the **mean log-likelihood**.

$$L = -\frac{1}{N}\|\bar{y} - X\bar{\beta}\|_2^2$$

N - observations.

$$= -\frac{1}{N}(\bar{y} - X\bar{\beta})^T(\bar{y} - X\bar{\beta})$$

$$\nabla L = -\frac{2}{N}\sum_{i=1}^{1} y_i - \bar{x}_i \cdot$$

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Numerical Minimization of OLS

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$$= -\frac{1}{N}(\bar{y} - X\bar{\beta})^T(\bar{y} - X\bar{\beta})$$

$$\nabla L = -\frac{2}{N}\sum_{i=1}^{N}(y_i - \bar{x}_i \cdot \bar{\beta})(\bar{x}_i)$$

$$= -\frac{2}{N}\underbrace{X}_{\text{data matrix}}^T(\bar{y} - X\bar{\beta})$$

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Numerical Minimization of OLS

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The Algorithm

The algorithm runs as follows:

- Pick a learning rate η
- Initialize $\vec{\beta}$ with a random guess
- Iterate

$$\vec{\beta} \leftarrow \vec{\beta} - \eta \frac{\partial \mathcal{L}}{\partial \vec{\beta}}$$

$$= \vec{\beta} + \frac{2\eta}{N} X^T [\vec{y} - X\vec{\beta}]$$

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Gradient Descent for Logistic Regression

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Gradient Descent for Logistic Regression

-8:23

Numerical Minimization of Logistic Loss

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$$\mathcal{L}(\vec{\beta}) = -\sum_i \left[\underbrace{y_i \log(\phi(\vec{x}_i \cdot \vec{\beta}))} + \underbrace{(1 - y_i) \log(1 - \phi(\vec{x}_i \vec{\beta}))} \right]$$

$$\phi(x) = \frac{1}{1+e^{-}}$$

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Numerical Minimization of Logistic Loss

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Numerical Minimization of Logistic Loss

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$$\phi(x) = \frac{1}{1+e^{-x}}$$

$$\phi(x) + \phi(-x) = 1 \quad \forall x.$$

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Hard Term

$$\frac{\partial}{\partial \beta_{j0}}[\log(\phi\,(\vec{x}_i \cdot \overrightarrow{\beta}))] =$$

$$\frac{\partial}{\partial \overrightarrow{\beta}}[\log(\phi\,(\vec{x}_i \overrightarrow{\beta}))] = \vec{x}_i^T(1 - \phi\,(\vec{x}_i \cdot \overrightarrow{\beta}))$$

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Hard Term

$$\frac{\partial}{\partial \beta_{j0}}[\log(\phi(\vec{x}_i \cdot \overrightarrow{\beta}))] = \frac{1}{\phi(\bar{x}_i \cdot \bar{\beta})} \frac{\partial}{\partial \beta_{j0}} \phi(\bar{x}_i \cdot \bar{\beta})$$

$$= \left(\frac{1+e^{-(\bar{x}_i \cdot \bar{\beta})}}{1}\right) \frac{\partial}{\partial \beta_{j0}} \left(\frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}\right)$$

$$= \left(1+e^{-(\bar{x}_i \cdot \bar{\beta})}\right) \frac{1}{\left(1+e^{-\bar{x}_i \cdot \bar{\beta}}\right)^2} e^{-\bar{x}_i \cdot \bar{\beta}} \left(-x_{ij0}\right)$$

$$\frac{\partial}{\partial \vec{\beta}}[\log(\phi(\vec{x}_i \overrightarrow{\beta}))] = \vec{x}_i^T(1 - \phi(\vec{x}_i \cdot \overrightarrow{\beta}))$$

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Hard Term

$$\frac{\partial}{\partial \beta_{j0}}[\log(\phi(\vec{x}_i \cdot \overrightarrow{\beta}))] = \frac{1}{\phi(\bar{x}_i \cdot \bar{\beta})} \frac{\partial}{\partial \beta_{j0}} \phi(\bar{x}_i \cdot \bar{\beta})$$

$$= \left(\frac{1+e^{-(\bar{x}_i \cdot \bar{\beta})}}{1}\right) \frac{\partial}{\partial \beta_{j0}} \left(\frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}\right)$$

$$= \left(1+e^{-(\bar{x}_i \cdot \bar{\beta})}\right) \frac{1}{\left(1+e^{-\bar{x}_i \cdot \bar{\beta}}\right)^2} e^{-\bar{x}_i \cdot \bar{\beta}} \left(-x_{ij0}\right)$$

$$\frac{\partial}{\partial \vec{\beta}}[\log(\phi(\vec{x}_i \overrightarrow{\beta}))] = \vec{x}_i^T(1 - \phi(\vec{x}_i \cdot \overrightarrow{\beta}))$$

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Hard Term

$$\frac{\partial}{\partial \beta_{j0}}[\log(\phi(\vec{x}_i \cdot \overrightarrow{\beta}))] = \frac{1}{\phi(\bar{x}_i \cdot \bar{\beta})} \frac{\partial}{\partial \beta_{j0}} \phi(\bar{x}_i \cdot \bar{\beta})$$

$$= \left(\frac{1+e^{-(\bar{x}_i \cdot \bar{\beta})}}{1}\right) \frac{\partial}{\partial \beta_{j0}} \left(\frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}\right)$$

$$= \cancel{\left(1+e^{-(\bar{x}_i \cdot \bar{\beta})}\right)} \frac{1}{\left(1+e^{-\bar{x}_i \cdot \bar{\beta}}\right)^{\cancel{2}}} e^{-\bar{x}_i \cdot \bar{\beta}} (-x_{ij0})$$

$$= \frac{1}{1+e^{+\cdot}}$$

$$\frac{\partial}{\partial \vec{\beta}}[\log(\phi(\vec{x}_i \overrightarrow{\beta}))] = \vec{x}_i^T(1-\phi(\vec{x}_i \cdot \overrightarrow{\beta}))$$

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Hard Term

$$\frac{\partial}{\partial \beta_{j0}}[\log(\phi(\vec{x}_i \cdot \overrightarrow{\beta}))] = \frac{1}{\phi(\bar{x}_i \cdot \bar{\beta})} \frac{\partial}{\partial \beta_{j0}} \phi(\bar{x}_i \cdot \bar{\beta})$$

$$= \left(\frac{1+e^{-(\bar{x}_i \cdot \bar{\beta})}}{1}\right) \frac{\partial}{\partial \beta_{j0}} \left(\frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}\right)$$

$$= \cancel{\left(1+e^{-(\bar{x}_i \cdot \bar{\beta})}\right)} \frac{1}{\left(1+e^{-\bar{x}_i \cdot \bar{\beta}}\right)^{\cancel{2}}} e^{-\bar{x}_i \cdot \bar{\beta}} (-x_{ij0})$$

$$= \frac{1}{1+e^{+\cdot}}$$

$$\frac{\partial}{\partial \vec{\beta}}[\log(\phi(\vec{x}_i \overrightarrow{\beta}))] = \vec{x}_i^T(1-\phi(\vec{x}_i \cdot \overrightarrow{\beta}))$$

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Hard Term

$$\frac{\partial}{\partial \beta_{jo}}[\log(\phi(\vec{x}_i \cdot \overrightarrow{\beta}))] = \frac{1}{\phi(\bar{x}_i \cdot \bar{\beta})} \frac{\partial}{\partial \beta_{jo}} \phi(\bar{x}_i \cdot \bar{\beta})$$

$$= \left(\frac{1+e^{-\bar{x}_i \cdot \bar{\beta}}}{1}\right) \frac{\partial}{\partial \beta_{jo}} \left(\frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}\right)$$

$$= \cancel{\left(1+e^{-\bar{x}_i \cdot \bar{\beta}}\right)} \frac{1}{\left(1+e^{-\bar{x}_i \cdot \bar{\beta}}\right)^{\cancel{2}}} e^{-\bar{x}_i \cdot \bar{\beta}} \left(-x_{ij_0}\right)$$

$$= \frac{1}{1+e^{+\bar{x}_i \cdot \bar{\beta}}} \left(x_{ij_0}\right)$$

$$\frac{\partial}{\partial \overrightarrow{\beta}}[\log(\phi(\vec{x}_i \overrightarrow{\beta}))] = \vec{x}_i^T(1 - \phi(\vec{x}_i \cdot \overrightarrow{\beta}))$$

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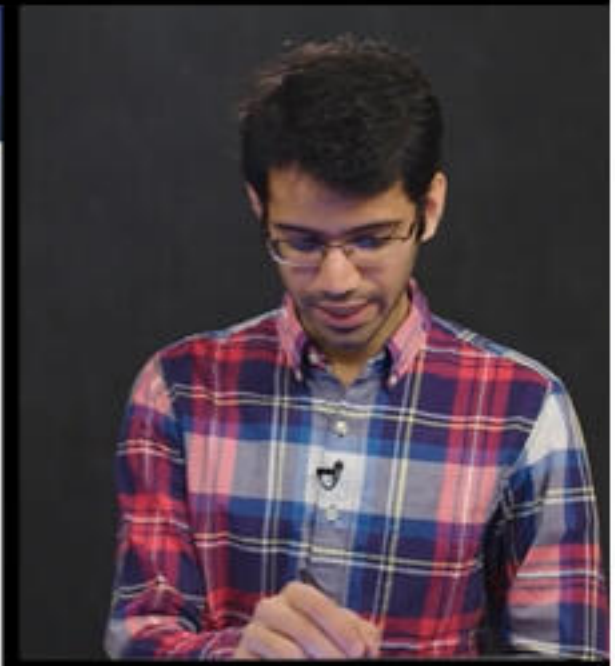

Hard Term

$$\frac{\partial}{\partial \beta_{jo}}[\log(\phi(\vec{x}_i \cdot \overrightarrow{\beta}))] = \frac{1}{\phi(\bar{x}_i \cdot \bar{\beta})} \frac{\partial}{\partial \beta_{jo}} \phi(\bar{x}_i \cdot \bar{\beta})$$

$$= \left(\frac{1+e^{-\bar{x}_i \cdot \bar{\beta}}}{1}\right) \frac{\partial}{\partial \beta_{jo}} \left(\frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}\right)$$

$$= \cancel{\left(1+e^{-\bar{x}_i \cdot \bar{\beta}}\right)} \frac{1}{\left(1+e^{-\bar{x}_i \cdot \bar{\beta}}\right)^{\cancel{2}}} e^{-\bar{x}_i \cdot \bar{\beta}} \left(-x_{ij_0}\right)$$

$$= \frac{1}{1+e^{+\bar{x}_i \cdot \bar{\beta}}} \left(x_{ij_0}\right)$$

$$\frac{\partial}{\partial \overrightarrow{\beta}}[\log(\phi(\vec{x}_i \overrightarrow{\beta}))] = \vec{x}_i^T(1 - \phi(\vec{x}_i \cdot \overrightarrow{\beta}))$$

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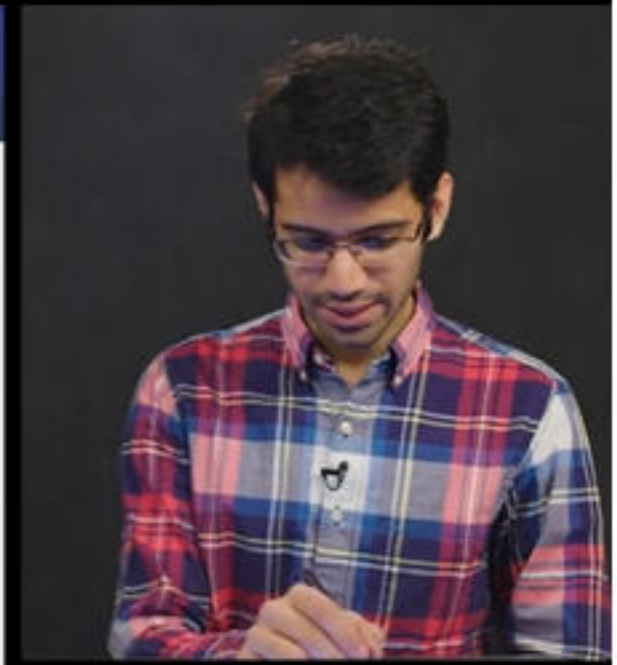

Hard Term

$$\frac{\partial}{\partial \beta_{j0}}[\log(\phi(\vec{x}_i \cdot \overrightarrow{\beta}))] = \frac{1}{\phi(\bar{x}_i \cdot \bar{\beta})} \frac{\partial}{\partial \beta_{j0}} \phi(\bar{x}_i \cdot \bar{\beta})$$

$$= \left(\frac{1+e^{-(\bar{x}_i \cdot \bar{\beta})}}{1}\right) \frac{\partial}{\partial \beta_{j0}} \left(\frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}\right)$$

$$= \left(\cancel{1+e^{-(\bar{x}_i \cdot \bar{\beta})}}\right) \frac{1}{\left(1+e^{-\bar{x}_i \cdot \bar{\beta}}\right)^2} e^{-\bar{x}_i \cdot \bar{\beta}} \left(-x_{ij0}\right)$$

$$= \frac{1}{1+e^{+\bar{x}_i \cdot \bar{\beta}}} \left(x_{ij0}\right) = \phi(-\bar{x}_i \cdot \bar{\beta})\, x_{ij0} =$$

$$\frac{\partial}{\partial \vec{\beta}}[\log(\phi(\vec{x}_i \overrightarrow{\beta}))] = \vec{x}_i^T (1 - \phi(\vec{x}_i \cdot \overrightarrow{\beta}))$$

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Hard Term

$$\frac{\partial}{\partial \beta_{j0}}[\log(\phi(\vec{x}_i \cdot \overrightarrow{\beta}))] = \frac{1}{\phi(\bar{x}_i \cdot \bar{\beta})} \frac{\partial}{\partial \beta_{j0}} \phi(\bar{x}_i \cdot \bar{\beta})$$

$$= \left(\frac{1+e^{-(\bar{x}_i \cdot \bar{\beta})}}{1}\right) \frac{\partial}{\partial \beta_{j0}} \left(\frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}\right)$$

$$= \left(\cancel{1+e^{-(\bar{x}_i \cdot \bar{\beta})}}\right) \frac{1}{\left(1+e^{-\bar{x}_i \cdot \bar{\beta}}\right)^{\cancel{2}}} e^{-\bar{x}_i \cdot \bar{\beta}} (-x_{ij0})$$

$$= \frac{1}{1+e^{+\bar{x}_i \cdot \bar{\beta}}} (x_{ij0}) = \phi(-\bar{x}_i \cdot \bar{\beta})\, x_{ij0} = (1-\phi(\bar{x}_i \cdot \bar{\beta}))\, x_{ij0}$$

$$\frac{\partial}{\partial \vec{\beta}}[\log(\phi(\vec{x}_i \overrightarrow{\beta}))] = \vec{x}_i^T (1 - \phi(\vec{x}_i \cdot \overrightarrow{\beta}))$$

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Hard Term 2

$$\frac{\partial}{\partial \beta}[\log(1 - \phi(\vec{x}_i \cdot \overrightarrow{\beta}))] = \frac{\partial}{\partial \beta} \log(\phi(-\vec{x}_i \cdot \vec{\beta}))$$

$$\frac{\partial}{\partial \vec{\beta}}[\log(1 - \phi(\vec{x}_i \overrightarrow{\beta}))] = -\vec{x}_i^T \phi(\vec{x}_i \cdot \overrightarrow{\beta})$$

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Hard Term 2

$$\frac{\partial}{\partial \beta}[\log(1-\phi(\vec{x}_i \cdot \overrightarrow{\beta}))] = \frac{\partial}{\partial \beta} \log\left(\phi(-\bar{x}_i \cdot \bar{\beta})\right)$$

$$= -x_i^T \left(1 - \phi(-\bar{x}_i \cdot \bar{\beta})\right)$$

$$=$$

$$\frac{\partial}{\partial \vec{\beta}}[\log(1-\phi(\vec{x}_i \overrightarrow{\beta}))] = -\vec{x}_i^T \phi(\vec{x}_i \cdot \overrightarrow{\beta})$$

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All Terms

$$\mathcal{L}(\vec{\beta}) = -\sum_i \left[y_i \log(\phi(\vec{x}_i \cdot \overrightarrow{\beta})) + (1 - y_i)\log(1 - \phi(\vec{x}_i \cdot \overrightarrow{\beta}))\right]$$

$$\frac{\partial \mathcal{L}(\vec{\beta})}{\partial \vec{\beta}} = -\sum_i y_i x_i^T \left(1 - \phi(\vec{x}_i \cdot \vec{\beta})\right) + 1 -$$

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All Terms

$$\mathcal{L}(\vec{\beta}) = -\sum_i \left[y_i \log(\phi(\vec{x}_i \cdot \overrightarrow{\beta})) + (1 - y_i)\log(1 - \phi(\vec{x}_i \cdot \overrightarrow{\beta}))\right]$$

$$\frac{\partial \mathcal{L}(\vec{\beta})}{\partial \vec{\beta}} = -\sum_i y_i x_i^T \left(1 - \phi(\vec{x}_i \cdot \vec{\beta})\right) + (1 - y_i)(-x_i^T)\, \phi(\vec{x}_i \cdot \vec{\beta})$$

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$$\mathcal{L}(\vec{\beta}) = -\sum_i \left[y_i \log(\phi(\vec{x}_i \cdot \vec{\beta})) + (1 - y_i)\log(1 - \phi(\vec{x}_i \cdot \vec{\beta}))\right]$$

$$\frac{\partial \mathcal{L}(\vec{\beta})}{\partial \vec{\beta}} = -\sum_i \left[y_i x_i^T \left(1 - \phi(\vec{x}_i \cdot \vec{\beta})\right) + (1 - y_i)(-x_i^T)\,\phi(\vec{x}_i \cdot \vec{\beta})\right]$$

$$= -\sum_i \left[y_i x_i^T - y_i x_i^T \phi(\vec{x}_i \cdot \vec{\beta}) + x_i^T y_i \phi(\vec{x}_i \cdot \vec{\beta}) - x_i^T \phi(\vec{x}_i \cdot \vec{\beta})\right]$$

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All Terms

$$\mathcal{L}(\vec{\beta}) = -\sum_i \left[y_i \log(\phi(\vec{x}_i \cdot \vec{\beta})) + (1 - y_i)\log(1 - \phi(\vec{x}_i \cdot \vec{\beta}))\right]$$

$$\frac{\partial \mathcal{L}(\vec{\beta})}{\partial \vec{\beta}} = -\sum_i \left[y_i x_i^T \left(1 - \phi(\vec{x}_i \cdot \vec{\beta})\right) + (1 - y_i)(-x_i^T)\,\phi(\vec{x}_i \cdot \vec{\beta})\right]$$

$$= -\sum_i \left[y_i x_i^T - \cancel{y_i x_i^T \phi(\vec{x}_i \cdot \vec{\beta})} + \cancel{x_i^T y_i \phi(\vec{x}_i \cdot \vec{\beta})} - x_i^T \phi(\vec{x}_i \cdot \vec{\beta})\right]$$

$$= -\sum_i x_i^T \left(y_i - \phi(\vec{x}_i \cdot \vec{\beta})\right)$$

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Topics

- Written Out Nicely
- A Note on Normalization
- The Algorithm

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Written Out Nicely

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}} = -X^T(\vec{y} - \Phi(X\vec{\beta}))$$

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Written Out Nicely

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}} = -X^T(\vec{y} - \phi(X\vec{\beta}))$$

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A Note on Normalization

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To work with different sized datasets, it is often better to divide everything by the number of observations N to get a **mean loss**.

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A Note on Normalization

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To work with different sized datasets, it is often better to divide everything by the number of observations N to get a **mean loss**.

This constant is carried through all the derivatives, as well as giving the final algorithm.

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The Algorithm

The algorithm runs as follows. Pick a learning rate n.

- Initialize $\vec{\beta}$ with a random guess.
- Iterate

$$\vec{\beta} \leftarrow \vec{\beta} - \eta \frac{\partial \mathcal{L}}{\partial \vec{\beta}} = \vec{\beta} + \frac{\eta}{N} X^T [\vec{y} - \phi(X\vec{\beta})].$$

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The Two Update Steps

$$\vec{\beta} \leftarrow \vec{\beta} + \underbrace{\frac{2\eta}{N} X^T}_{\text{OLS}} \underbrace{[\vec{y} - X\vec{\beta}]}_{\text{residual error}}$$

vs.

$$\vec{\beta} \leftarrow \vec{\beta} + \underbrace{\frac{\eta}{N} X^T}_{\text{Logistic}} [\underbrace{\vec{y} - \phi(X\vec{\beta})}_{\text{error}}]$$

$\in \{0,1$

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The Two Update Steps

$$\vec{\beta} \leftarrow \vec{\beta} + \underbrace{\frac{2\eta}{N}}_{} X^T \underbrace{[\vec{y} - X\vec{\beta}]}_{\text{residual error}}$$

OLS

vs.

$$\vec{\beta} \leftarrow \vec{\beta} + \underbrace{\frac{\eta}{N}}_{} X^T [\vec{y} - \phi(X\vec{\beta})]$$

Logistic

error

$\in \{0, 1$

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The Two Update Steps

$$\vec{\beta} \leftarrow \vec{\beta} + \underbrace{\frac{2\eta}{N} X^T}_{\text{OLS}} \underbrace{[\vec{y} - X\vec{\beta}]}_{\text{residual error}}$$

vs.

$$\vec{\beta} \leftarrow \vec{\beta} + \underbrace{\frac{\eta}{N} X^T}_{\text{Logistic}} [\underbrace{\vec{y} - \phi(X\vec{\beta})}_{\text{error}}]$$

$\in \{0, 1\}$

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Regularization

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OLS :

Regularization, $\mathcal{L} = \|\bar{y} - X\bar{\beta}\|_2^2 + \delta^2 \|\beta\|_{2/1}^{2/1}$

Logistic :

Reg, $\mathcal{L} = \underbrace{\mathcal{L}(\beta)}_{\text{logistic loss function}} + \delta^2 \|\beta\|_{2/1}^{2/1}$

Ridge ← uniform penalization

LAS

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The Softmax

$$P(Y = c_j \mid x_i) = \frac{e^{\bar{\beta}_j \cdot \bar{x}_i}}{\sum_{j=1}^{M} e^{\bar{\beta}_j \cdot \bar{x}_i}}$$

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The Softmax

$$P(Y = c_j \mid x_i) = \frac{e^{\bar{\beta}_j \cdot \bar{x}_i}}{\sum_{j=1}^{M} e^{\bar{\beta}_j \cdot \bar{x}_i}}$$

$y \in \{1, \dots, M\}$

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The Softmax

$$P(Y = c_j \mid x_i) = \frac{e^{\bar{\beta}_j \cdot \bar{x}_i}}{\sum_{j=1}^{M} e^{\bar{\beta}_j \cdot \bar{x}_i}}$$

$y \in \{1, \dots, M\}$

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The Softmax

$$P(Y = c_j \mid x_i) = \frac{e^{\bar{\beta}_j \cdot \bar{x}_i}}{\sum_{j=1}^{M} e^{\bar{\beta}_j \cdot \bar{x}_i}}$$

$y \in \{1, \dots, M\}$

S

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Comparison with Logistic in the Case of Two Types

$$P(Y=1 \mid \bar{x}_i) = \frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}$$

$$P(Y=1 \mid \bar{x}_i) = \frac{e^{\bar{x}_i \cdot \bar{\beta}_1}}{e^{\bar{x}_i \cdot \bar{\beta}_1} + e^{\bar{x}_i \cdot \bar{\beta}}}$$

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Comparison with Logistic in the Case of Two Types

$$P(Y=1 \mid \bar{x}_i) = \frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}$$

$$P(Y=1 \mid \bar{x}_i) = \frac{e^{\bar{x}_i \cdot \bar{\beta}_1} \times e^{-\bar{x} \cdot \bar{\beta}_1}}{e^{\bar{x}_i \cdot \bar{\beta}_1} + e^{\bar{x}_i \cdot \bar{\beta}_2} \times} \qquad Y \in \{1, 2\}$$

$$= \frac{1}{1+e^{-\bar{x}_i \cdot (\bar{\beta}_1 - \bar{\beta}_2)}}$$

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Comparison with Logistic in the Case of Two Types

$$\boxed{P(Y=1 \mid \bar{x}_i) = \frac{1}{1+e^{-\bar{x}_i \cdot \bar{\beta}}}}$$

$Y \in \{1,2\}$

$$P(Y=1 \mid \bar{x}_i) = \frac{e^{\bar{x}_i \cdot \bar{\beta}_1} \times e^{-\bar{x} \cdot \bar{\beta}_1}}{e^{\bar{x}_i \cdot \bar{\beta}_1} + e^{\bar{x}_i \cdot \bar{\beta}_2} \times}$$

$$= \frac{1}{1+e^{-\bar{x}_i \cdot (\bar{\beta}_1 - \bar{\beta}_2)}}$$

$\beta \equiv \beta_1 - \beta_2$

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The Gradients

This can all be computed as before. Let's all avoid the pain. First you need the classification probabilities:

$$\underbrace{\pi_{i,j}}_{\text{probabilities (observation } i\text{, class } j)} = \frac{e^{\overrightarrow{x_i}\vec{\beta}_j}}{\sum_k e^{\overrightarrow{x_i}\vec{\beta}_k}}, \vec{\pi}_j = \begin{pmatrix} \pi_{1,j} \\ \vdots \\ \pi_{N,j} \end{pmatrix}$$

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The Gradients

Once you compute the loss and take the derivative, you see that:

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}_j} = -X^T(\vec{y_j} - \vec{\pi}_j).$$

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The Gradients

Once you compute the loss and take the derivative, you see that:

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}_j} = -X^T(\vec{y_j} - \vec{\pi}_j).$$

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The Gradients

Once you compute the loss and take the derivative, you see that:

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}_j} = -X^T(\vec{y}_j - \vec{\pi}_j).$$

compare: $-X^T(\bar{y} - \underbrace{\Phi(X\bar{\beta})}_{\text{er}})$

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The Gradients

Once you compute the loss and take the derivative, you see that:

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}_j} = -X^T(\overbrace{\vec{y_j} - \vec{\pi}_j}^{\text{error}}).$$

compare: $-X^T(\underbrace{\bar{y} - \sigma(X\bar{\beta})}_{\text{error}})$

$$\bar{y}_i = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{bmatrix}$$

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The Gradients

Once you compute the loss and take the derivative, you see that:

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}_j} = -X^T(\overbrace{\vec{y}_j - \vec{\pi}_j}^{\text{error}}).$$

compare: $-X^T(\underbrace{\vec{y} - \vec{\pi}(X\vec{\beta})}_{\text{error}})$

$$\vec{y}_i = \begin{array}{c} \\ \\ j^{th} \\ \\ \\ \end{array}\begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{bmatrix} \leftarrow y_i = j$$

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Gradient Descent Algorithm

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And thus the algorithm is largely unchanged.

0 Initialize η

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Gradient Descent Algorithm

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And thus the algorithm is largely unchanged.

① Initialize η, random choice for $(\bar{\beta}_1, \ldots, \bar{\beta}_M)$

② $\bar{\beta}_j \leftarrow \bar{\beta}_j + \eta$

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Gradient Descent Algorithm

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And thus the algorithm is largely unchanged.

① Initialize η, random choice for $(\bar{\beta}_1, \ldots, \bar{\beta}_M)$

② $$\boxed{\bar{\beta}_j \leftarrow \bar{\beta}_j + \frac{\eta}{N} X^T (\bar{y}_j - \bar{\pi}_j)}$$

GD to solve sa

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A Warning

Learning rate, η $\longrightarrow$ small $\Rightarrow$ long time to converge

large $\Rightarrow$ convergence not happen

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A Warning

Learning rate, η → small ⇒ long time to converge

large ⇒ convergence not happen

monitor loss function

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A Warning

Learning rate, η → small ⇒ long time to converge

large ⇒ convergence not happen

monitor loss function

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A Warning

Learning rate, η → small ⇒ long time to converge

large ⇒ convergence not happen

→ monitor loss function

→ normalizing correctly $\left(\frac{1}{N}\right)$

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All Gradient Descents Are The Same

OLS
Logistic
Softmax

$\rightarrow$

$\bar{\beta}$ random

$\bar{\beta}$ —

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Optimization

There is no limit on how stochastic gradient descent (SGD) can be modified to try to avoid pitfalls.

Optimization

Which method will work best depends on your data, and the only way to really know for sure is to **try** them out and select the method that produces the **best test loss**.

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Optimization

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Honestly, many machine learning practitioners just pick a favorite.

For example, some practitioners like the comfort of a large body of literature with SGD.

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Images

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Numerical Methods for Optimization

In this final section, we explore optimization models that are more efficient than the logistic gradient descent method. We also explain how to address the learning rate issue and explore a few more optimization hacks that are based on the current and previous classifications of gradients.

The following topics will be covered:

- Numerical methods for optimizing learning models
- A review of the gradient descent method
- Other optimization techniques
  - Newton's method
  - Stochastic gradient descent
  - Mini-batch algorithm
- Optimization techniques based on current and historical gradient values
  - Momentum
  - AdaGrad

Review

- Gradient Descent

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Other Methods

- Other Optimization Methods

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Newton's Method

- Definition of Newton's Method
- Recall: The Hessian

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Newton's Method for Ordinary Least Squares (OLS)

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- Gradients
- Hessians
- The Update Step

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Logistic Regression

- Deriving the Update Step

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Issues With Newton's Method

- An Issue with Newton's Method

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Stochastic Gradient Descent

- The Idea
- What Order?
- Approximate Computational Complexity
- The Big Gains

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Stochastic Gradient Descent

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- The Idea
- What Order?
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- The Big Gains

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Mini Batch

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- Idea
- Pictorially
- A Note on the Use of Noise
- Update Step (and Regularization)
- Definition of Epoch

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Momentum

- A Useful Hack
- Note $\alpha = 0$
- Benefits
- Downsides

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AdaGrad

- The Expression
- Benefits
- Downsides

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AdaGrad

- The Expression
- Benefits
- Downsides

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Optimization in Practice

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- Additional Optimization Methods

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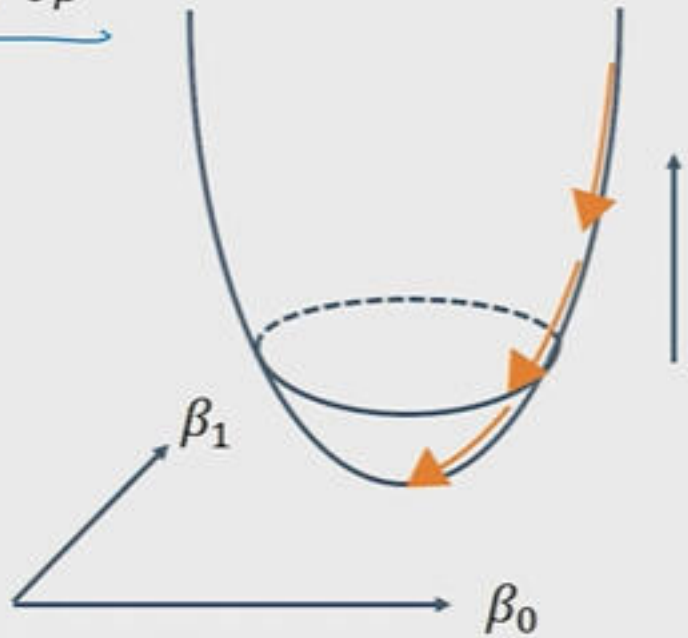
Gradient Descent

- Generate random parameters $\vec{\beta}$
- Iterate: $\vec{\beta} \leftarrow \vec{\beta} - \eta \frac{\partial \mathcal{L}}{\partial \vec{\beta}}$



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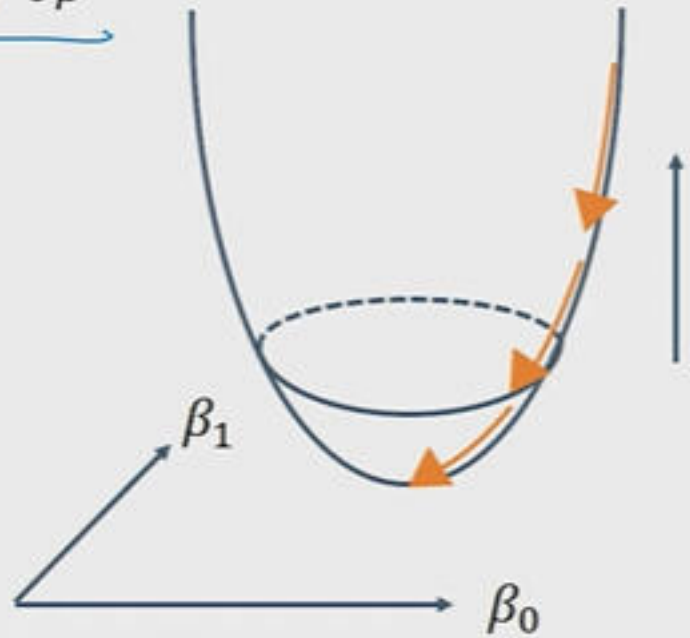
Gradient Descent

- Generate random parameters $\vec{\beta}$
- Iterate: $\vec{\beta} \leftarrow \vec{\beta} - \eta \frac{\partial \mathcal{L}}{\partial \vec{\beta}}$



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For Regression

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}} = -X^T(\bar{y} - X\bar{\beta})$$

$$= -X^T(\bar{y} - f(X\bar{\beta}))$$

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For Regression

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}} = -X^T(\bar{y} - X\bar{\beta})$$

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}} = -X^T(\bar{y} - f(X\bar{\beta}))$$

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For Regression

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}} = -X^T(\bar{y} - X\bar{\beta})$$

$$\frac{\partial \mathcal{L}}{\partial \bar{\beta}} = -X^T(\bar{y} - \underbrace{f}_{\text{link function}}(X\bar{\beta}))$$

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For Regression

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}} = -X^T(\bar{y} - X\bar{\beta})$$

$$\frac{\partial \mathcal{L}}{\partial \bar{\beta}} = -X^T(\bar{y} - \underbrace{f}_{\text{link function}}(X\bar{\beta}))$$

$$f(x) = x$$

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For Regression

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}} = -X^T(\bar{y} - X\bar{\beta})$$

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}} = -X^T(\bar{y} - \underbrace{f}_{\text{link function}}(X\bar{\beta}))$$

$$f(x) = x \leftarrow \text{OLS}$$

$$f(x) = \frac{1}{1+e^{-x}} \leftarrow$$

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For Regression

$$\frac{\partial \mathcal{L}}{\partial \vec{\beta}} = -X^T(\bar{y} - X\bar{\beta})$$

$$\frac{\partial \mathcal{L}}{\partial \bar{\beta}} = -X^T(\bar{y} - \underbrace{f}_{\text{link function}}(X\bar{\beta}))$$

$$f(x) = x \leftarrow \text{OLS}$$

$$f(x) = \frac{1}{1+e^{-x}} \leftarrow \text{Logistic}$$

$$f(x) = e^x \leftarrow \text{Poisson}$$

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Other Optimization Methods

In this video, we briefly discuss other optimization models that are reliant on the gradient descent technique but have a modification.

Optimization techniques based on gradient descent:

- Newton's method ← uses a higher order derivative.
- Stochastic gradient descent ← randomly selects one data point in each iteration.
- Mini-batch gradient descent ← randomly selects data points from set of m-data points.
- Momentum gradient descent ← incorporates additional parameter to capture historical gradients.
- AdaGrad ← modifies learning rate to capture historical gradient.

Other Optimization Methods

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1. Newton's method ← higher order derivative

2. Stochastic Gradient Descent ← random selection of single data point for update.

3. Mini-batch Gradient Descent ← 'm' data points → batch

4. Momentum ← incorporate additional parameter to capture historical gradients

5. AdaGrad ← modifies learning rate to capture historical gradients.

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Other Optimization Methods

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1. Newton's method ← higher order derivative
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3. Mini-batch Gradient Descent ← 'm' data points → batch
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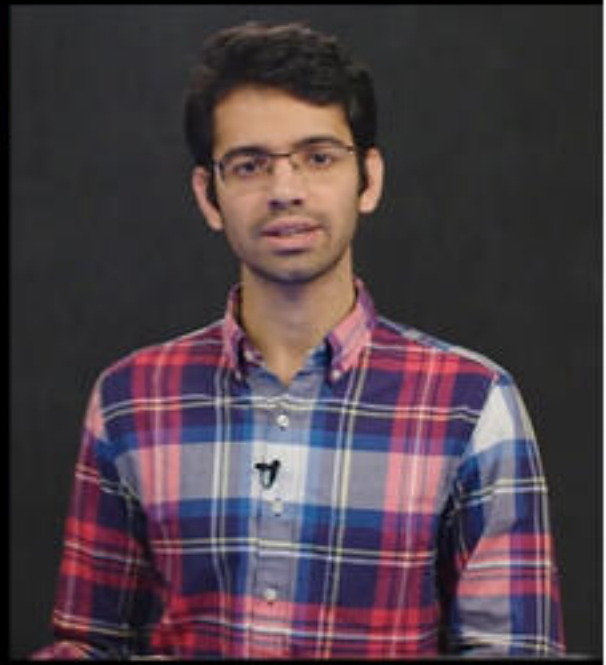

-0:13

Other Optimization Methods

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1. Newton's method ← higher order derivative

2. Stochastic Gradient Descent ← random selection of single data point for update.

3. Mini-batch Gradient Descent ← 'm' data points → batch

4. Momentum ← incorporate additional parameter to capture historical gradients

5. AdaGrad ← modifies learning rate to capture historical gradien

-0:14

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Definition

$$\vec{\beta} = \vec{\beta} - \underbrace{[HL(\vec{\beta})]^{-1}}\frac{\partial \mathcal{L}}{\partial \vec{\beta}}$$

speeding up convergence
due to higher order derivative

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Recall: The Hessian

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matrix: $$H\mathcal{L}(\bar{\beta}) = \frac{\partial}{\partial \bar{\beta}}(\nabla \mathcal{L}) = \frac{\partial}{\partial \bar{\beta}}\underbrace{\left(\frac{\partial \mathcal{L}}{\partial \bar{\beta}}\right)}_{\text{gradient}}$$

M ind vars $\rightarrow (M+1)$

N observations

$$H\mathcal{L}(\bar{\beta}) = \begin{bmatrix} \frac{\partial \mathcal{L}}{\partial \beta_0 \partial \beta_0} & \cdots & \frac{\partial \mathcal{L}}{\partial \beta_0 \partial \beta_M} \\ & & \\ & & \end{bmatrix}_{\times M1}$$

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Newton's Method for Ordinary Least Squares (OLS)

-4:09

Gradients

$$\nabla_{\bar{\beta}} \mathcal{L} = -2 \underbrace{X^T}_{\text{data matrix}} \underbrace{(\bar{y} - X\bar{\beta})}_{\text{residual error}}$$

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The Update Step

$$\bar{\beta} \leftarrow \bar{\beta} - \left(H L(\beta)\right)^{-1} \left(\nabla_{\beta} L\right)$$

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The Update Step

$$\bar{\beta} \leftarrow \bar{\beta} - (H L(\beta))^{-1} (\nabla_{\beta} L)$$

$$\bar{\beta} - (2X^T X)^{-1} ($$

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The Update Step

$$\bar{\beta} \leftarrow \bar{\beta} - \left(H L(\bar{\beta})\right)^{-1} \left(\nabla_{\bar{\beta}} L\right)$$

$$= \bar{\beta} - \left(\cancel{2} X^T X\right)^{-1} \left(-\cancel{2} X^T (\bar{y} - X\bar{\beta})\right)$$

$$= \bar{\beta} + (X^T X)^{-1} \left(X^T y - X^T X \beta\right)$$

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The Update Step

$$\bar{\beta} \leftarrow \bar{\beta} - (H L(\bar{\beta}))^{-1} (\nabla_{\bar{\beta}} L)$$

$$= \bar{\beta} - (2X^T X)^{-1} \left(-2X^T(\bar{y} - X\bar{\beta})\right)$$

$$= \bar{\beta} + (X^T X)^{-1} \left(X^T y - X^T X \beta\right)$$

$$= \bar{\beta} + (X^T X)^{-1} X^T y - (X^T X)^{-1} (X^T X)$$

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The Update Step

$$\bar{\beta} \leftarrow \bar{\beta} - (H L(\bar{\beta}))^{-1} (\nabla_{\bar{\beta}} L)$$

$$= \bar{\beta} - (\cancel{2} X^T X)^{-1} \left(-\cancel{2} X^T (\bar{y} - X\bar{\beta}) \right)$$

$$= \bar{\beta} + (X^T X)^{-1} \left(X^T y - X^T X \bar{\beta} \right)$$

$$= \cancel{\bar{\beta}} + (X^T X)^{-1} X^T y - \cancel{(X^T X)^{-1} (X^T X) \bar{\beta}}$$

$$\boxed{\bar{\beta} = (X^T X)^{-1} X^T y}$$

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The Update Step

- This is the same as our original closed-form solution!

- For OLS, the Newton's method is exact in **one step**, and is an **alternate way** to derive the exact solutions that have been previously discussed.

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Deriving the Update Step

$$\nabla_\beta \mathcal{L} = -X^T\left(\bar{y} - \Phi(X\bar{\beta})\right)$$

$$H\mathcal{L}(\beta) = \frac{\partial}{\partial \beta}\left(-X^T\left(\underbrace{\bar{y}}_{0} - \Phi(X\bar{\beta})\right)\right)$$

$$= X^T \Phi(X\bar{\beta}) \circ (\bar{1}$$

$$\Phi(x) = \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_N) \end{bmatrix}$$

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Deriving the Update Step

$$\nabla_\beta \mathcal{L} = -X^T\left(\bar{y} - \Phi(X\bar{\beta})\right)$$

$$H\mathcal{L}(\beta) = \frac{\partial}{\partial \beta}\left(-X^T\left(\bar{y} - \Phi(X\bar{\beta})\right)\right)$$

$$= X^T \Phi(X\bar{\beta}) \circ \left(\bar{1} - \Phi(X\bar{\beta})\right) X$$

element-wise product

$$\Phi(x) = \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_N) \end{bmatrix}$$

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Deriving the Update Step

$$\nabla_\beta \mathcal{L} = -X^T(\bar{y} - \Phi(X\bar{\beta}))$$

$$H\mathcal{L}(\beta) = \frac{\partial}{\partial \beta}\left(-X^T(\bar{y} - \Phi(X\bar{\beta}))\right)$$

$$= X^T \Phi(X\bar{\beta}) \circ (\bar{1} - \Phi(X\bar{\beta}))X$$

element-wise product

$$\Phi(x) = \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_N) \end{bmatrix}$$

$$\left[\phi(\bar{x}_i \cdot \bar{\beta})(1 - \phi(\bar{x}_i \cdot \bar{\beta})) \right]$$

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Deriving the Update Step

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$$\nabla_\beta \mathcal{L} = -X^T(\bar{y} - \Phi(X\bar{\beta}))$$

$$H\mathcal{L}(\beta) = \frac{\partial}{\partial \beta}\left(-X^T(\bar{y} - \Phi(X\bar{\beta}))\right)$$

$$= X^T \Phi(X\bar{\beta}) \circ (\bar{1} - \Phi(X\bar{\beta}))\, X$$

element-wise product

vector of 1's

$$\Phi(x) = \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_N) \end{bmatrix}$$

$$\phi(\bar{x}_i \cdot \bar{\beta})\,(1 - \phi(\bar{x}_i \cdot \bar{\beta}))$$

$$\beta \leftarrow \beta - (H\mathcal{L}(\beta))^{-1} \nabla_\beta \mathcal{L}$$

$$= \beta - X^T \Phi(X\bar{\beta}) \circ (\bar{1} - \Phi(X$$

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Deriving the Update Step

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$$\nabla_\beta \mathcal{L} = -X^T\left(\bar{y} - \Phi(X\bar{\beta})\right)$$

$$H\mathcal{L}(\beta) = \frac{\partial}{\partial \beta}\left(-X^T\left(\bar{y} - \Phi(X\bar{\beta})\right)\right)$$

$$= X^T \Phi(X\bar{\beta}) \circ \left(\bar{1} - \Phi(X\bar{\beta})\right) X$$

element-wise product

vector of $\begin{pmatrix}1\\ \vdots \\ 1\end{pmatrix}$

$$\Phi(x) = \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_N) \end{bmatrix}$$

$$\left[\phi(\bar{x}_i \cdot \bar{\beta})\left(1 - \phi(\bar{x}_i \cdot \bar{\beta})\right)\right]$$

$$\beta \leftarrow \beta - \left(H\mathcal{L}(\beta)\right)^{-1} \nabla_\beta \mathcal{L}$$

$$= \beta - \left[X^T \Phi(X\bar{\beta}) \circ \left(\bar{1} - \Phi(X\bar{\beta})\right) X\right]^{-1}$$

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Deriving the Update Step

$$\nabla_\beta \mathcal{L} = -X^T(\bar{y} - \Phi(X\bar{\beta}))$$

$$H\mathcal{L}(\beta) = \frac{\partial}{\partial \beta}\left(-X^T(\bar{y} - \Phi(X\bar{\beta}))\right)$$

$$= X^T \Phi(X\bar{\beta}) \circ \left(\bar{1} - \Phi(X\bar{\beta})\right) X$$

element-wise product

vector of 1's

$$\Phi(x) = \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_N) \end{bmatrix}$$

$$\left[\phi(\bar{x}_i \cdot \bar{\beta})\left(1 - \phi(\bar{x}_i \cdot \bar{\beta})\right)\right]$$

$$\beta \leftarrow \beta - \left(H\mathcal{L}(\beta)\right)^{-1} \nabla_\beta \mathcal{L}$$

$$= \beta + \left[X^T \Phi(X\bar{\beta}) \circ \left(\bar{1} - \Phi(X\bar{\beta})\right) X\right]^{-1} X^T(\bar{y} - \Phi$$

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Deriving the Update Step

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$$\nabla_\beta \mathcal{L} = -X^T(\bar{y} - \Phi(X\bar{\beta}))$$

$$H\mathcal{L}(\beta) = \frac{\partial}{\partial \beta}\left(-X^T(\bar{y} - \Phi(X\bar{\beta}))\right)$$

$$= X^T \Phi(X\bar{\beta}) \circ \left(\bar{1} - \Phi(X\bar{\beta})\right) X$$

element-wise product

vector of 1's

$$\Phi(x) = \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_N) \end{bmatrix}$$

$$\left[\phi(\bar{x}_i \cdot \bar{\beta})\left(1 - \phi(\bar{x}_i \cdot \bar{\beta})\right)\right]$$

$$\beta \leftarrow \beta - \left(H\mathcal{L}(\beta)\right)^{-1} \nabla_\beta \mathcal{L}$$

$$= \beta + \left[X^T \Phi(X\bar{\beta}) \circ \left(\bar{1} - \Phi(X\bar{\beta})\right) X\right]^{-1} X^T(\bar{y} - \Phi(X\bar{\beta}))$$

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An Issue with Newton's Method

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Slow

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An Issue with Newton's Method

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Slow

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An Issue with Newton's Method

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Slow

quadratic dependence # fea

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An Issue with Newton's Method

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Slow

quadratic dependence # features.

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Stochastic Gradient Descent

-11:53

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Stochastic Gradient Descent

-11:54

Topics

- The Idea
- What Order?
  - Cycle through
  - Random elements
  - Shuffle then cycle through
- Approximate Computational Complexity
- The Big Gains

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The Idea

$$\bar{\beta} \leftarrow \bar{\beta} - \underbrace{\eta}_{\text{learning rate}} \underbrace{(\nabla_{\bar{\beta}} \mathcal{L})}_{\text{gradient of } \mathcal{L}}$$

$\longrightarrow$ defined on $X, \bar{y}$

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The Idea

$$\bar{\beta} \leftarrow \bar{\beta} - \underbrace{\eta}_{\text{learning rate}} \underbrace{\left(\nabla_{\bar{\beta}} \mathcal{L}\right)}_{\text{gradient of } \mathcal{L}}$$

$\longrightarrow$ defined on $X, \bar{y}$

GD:

$$\Big\downarrow \text{OLS}$$

$$\bar{\beta} \leftarrow \bar{\beta} + X^T(\bar{y} - X\bar{\beta})$$

SGD : single observation in each update

β

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The idea

$$\bar{\beta} \leftarrow \bar{\beta} - \underbrace{\eta}_{\text{learning rate}} \underbrace{\left(\nabla_{\bar{\beta}} \mathcal{L}\right)}_{\text{gradient of } \mathcal{L}}$$

$\longrightarrow$ defined on $X, \bar{y}$

GD:

OLS

$$\bar{\beta} \leftarrow \bar{\beta} + \eta X^T (\bar{y} - X\bar{\beta})$$

SGD : single observation in each update.

$$\boxed{\bar{\beta} \leftarrow \bar{\beta} + \eta\, \bar{x}_i^T (y_i - \bar{x}_i \cdot \bar{\beta})}$$

observation : one at a time.

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The idea

$$\bar{\beta} \leftarrow \bar{\beta} - \underbrace{\eta}_{\text{learning rate}} \underbrace{\left(\nabla_{\bar{\beta}} \mathcal{L}\right)}_{\text{gradient of } \mathcal{L}} \longrightarrow \text{defined on } X, \bar{y}$$

GD:

OLS

$$\bar{\beta} \leftarrow \bar{\beta} + \eta X^T (\bar{y} - X\bar{\beta})$$

SGD : single observation in each update.

$$\boxed{\bar{\beta} \leftarrow \bar{\beta} + \eta\, \bar{x}_i^T (y_i - \bar{x}_i \cdot \bar{\beta})}$$

observation : one at a time.

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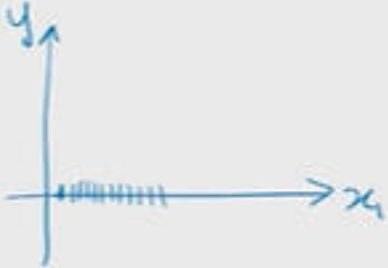
Order: Cycle Through?

- Not robust to patterns in the dataset



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Order: Random Elements?

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- You'll see some data points **many times** before you see others even **once**.

1 2 3 . . . . . N

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Order: Shuffle Then Cycle Through?

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- Shuffle, then cycle through, and repeat
- Take advantage of the benefits of both

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Order: Shuffle Then Cycle Through?

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- Shuffle, then cycle through, and repeat
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Order: Shuffle Then Cycle Through?

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- Shuffle, then cycle through, and repeat
- Take advantage of the benefits of both

randomization cycling.

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Approximate Computational Complexity

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① Computational complexity of each iteration

② # iterations needed to reach an accuracy of ϵ.

GD	SGD
N	1

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Approximate Computational Complexity

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① Computational complexity of each iteration

② # iterations needed to reach an accuracy of ϵ

③ Comp complexity to reach

GD	SGD
N	1
$\log(1/\epsilon)$	$1/\epsilon$

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Approximate Computational Complexity

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① Computational complexity of each iteration

② # iterations needed to reach an accuracy of ϵ

③ Comp complexity to reach accuracy

GD	SGD
N	1
$\log(1/\epsilon)$	$1/\epsilon$

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Approximate Computational Complexity

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① Computational complexity of each iteration

② # iterations needed to reach an accuracy of ϵ

③ Comp complexity to reach accuracy

GD	SGD
N	1
$\log(1/\epsilon)$	$1/\epsilon$
$N \log(1/\epsilon)$	$1/\epsilon$

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Gain: Work and Accuracy

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Work and accuracy are directly related

No longer conflate the notions of the amount of data and desired accuracy

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Gain: Work and Accuracy

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Work and accuracy are directly related

No longer conflate the notions of the amount of data and desired accuracy

SGD ϵ : $(1/\epsilon)$

GD ϵ : $N \log(1/\epsilon)$

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Gain: Work and Accuracy

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Work and accuracy are directly related

No longer conflate the notions of the amount of data and desired accuracy

SGD ϵ : $(1/\epsilon)$

GD ϵ : $\underline{N} \log(1/\epsilon)$

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Gain: Work and Accuracy

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Work and accuracy are directly related

No longer conflate the notions of the amount of data and desired accuracy

SGD ϵ : $(1/\epsilon)$

GD ϵ : $\underline{N} \log(1/\epsilon))$

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Gain: Online Learning

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Can be done *online*

→ iteration only uses a single observation

→ assumption: distribution of data doesn't change w/time

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Gain: Online Learning

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Can be done *online*

→ iteration only uses a single observation

→ assumption: distribution of data doesn't change w/time

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Update Step (and Regularization)

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$$\frac{\mathcal{L}}{N} = \underbrace{\frac{1}{N}\|\bar{y} - X\bar{\beta}\|_2^2}_{\mathcal{L}_1} + \underbrace{\frac{\delta_2^2}{N}\|\beta\|_2^2}_{\mathcal{L}_2} \longleftarrow \text{Ridge reg.}$$

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Update Step (and Regularization)

$$\frac{\mathcal{L}}{N} = \underbrace{\frac{1}{N}\|\bar{y} - X\bar{\beta}\|_2^2}_{\mathcal{L}_1} + \underbrace{\frac{\delta_2^2}{N}\|\beta\|_2^2}_{\mathcal{L}_2} \longleftarrow \text{Ridge reg.}$$

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Update Step (and Regularization)

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$$\frac{\mathcal{L}}{N} = \underbrace{\frac{1}{N}\|\bar{y} - X\bar{\beta}\|_2^2}_{\substack{\mathcal{L}_1 \\ \text{error}}} + \underbrace{\frac{\delta_2^2}{N}\|\beta\|_2^2}_{\mathcal{L}_2} \longleftarrow \text{Ridge reg.}$$

$$\underbrace{\frac{1}{m}}\underbrace{\|\bar{y} - X\bar{\beta}\|_2^2}_{\text{error}}$$

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Update Step (and Regularization)

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$$\frac{\mathcal{L}}{N} = \underbrace{\frac{1}{N}\|\bar{y} - X\bar{\beta}\|_2^2}_{\substack{\mathcal{L}_1 \\ \text{error}}} + \underbrace{\left(\frac{\delta_2^2}{N}\|\beta\|_2^2\right)}_{\mathcal{L}_2} \longleftarrow \text{Ridge reg.}$$

$$\underbrace{\frac{1}{m}}\underbrace{\|\bar{y} - X\bar{\beta}\|_2^2}_{\text{error}} + \frac{m}{N}\delta_2^2\|\beta\|_2^2$$

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Update Step (and Regularization)

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$$\frac{\mathcal{L}}{N} = \underbrace{\frac{1}{N}\|\bar{y} - X\bar{\beta}\|_2^2}_{\substack{\mathcal{L}_1 \\ \text{error}}} + \underbrace{\left(\frac{\delta_2^2}{N}\|\beta\|_2^2\right)}_{\mathcal{L}_2} \longleftarrow \text{Ridge reg.}$$

$$\mathcal{L}_{m.b} = \underbrace{\frac{1}{m}}\underbrace{\|\bar{y} - X\bar{\beta}\|_2^2}_{\text{error}} + \frac{m}{N}\delta_2^2\|\beta\|_2^2$$

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Definition of *Epoch*

SGD : 1 obs
M.B : m obs.
GD : N obs

update step

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Definition of *Epoch*

SGD : 1 obs
M.B : m obs.
GD : N obs

update step

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Definition of *Epoch*

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SGD : 1 obs
M.B : m obs.
GD : N obs

} update step

Epoch : Number of iterations to pass over the entire dataset.

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Definition of *Epoch*

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M.B : m obs.
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SGD : N iterations
MB.

} 1 epoch

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SGD : N iterations
MB

} 1 epoch

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M.B : m obs.
GD : N obs.

} update step

Epoch : Number of iterations to pass over the entire dataset.

SGD : N iterations
MB

} 1 epoch

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Definition of *Epoch*

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SGD : 1 obs
M.B : m obs.
GD : N obs.

} update step

Epoch : Number of iterations to pass over the entire dataset.

SGD : N iterations
MB :

} 1 epoch

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Definition of *Epoch*

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SGD : 1 obs
M.B : m obs.
GD : N obs.

} update step

Epoch : Number of iterations to pass over the entire dataset.

SGD : N iterations
MB : $\frac{N}{m}$ iterations
GD : 1 iterati

} 1 epoch

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Per Epoch is Optimal to Compare

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For most relatives to gradient descent, it takes almost the exact same clock-time to compute an epoch (for example, up to about 10 percent).

Thus, per-epoch improvement in loss can be used as a proxy for how long it will take you to learn something.

A Useful Hack

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GD: $\bar{\beta} \leftarrow \underbrace{\bar{\beta} - \eta(\nabla L)}$

Momentum: $\bar{\beta} \leftarrow \beta + \bar{v}$

$$\bar{v} \leftarrow (1-\alpha)\underbrace{(-\eta \nabla L)}_{GD} + \alpha \bar{v}$$

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Note

$\alpha = 0$

$$\bar{v} \leftarrow (1-\alpha)\underbrace{(-\eta \nabla L)} + \underbrace{\alpha \bar{v}}_{\to 0 \text{ when } \alpha = 0}$$

$$\bar{\beta} \leftarrow \bar{\beta} + \bar{v}$$

when $\alpha = 0$, Momentum $\longrightarrow$ GD

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Note

$\alpha = 0$

$$\bar{v} \leftarrow (1-\alpha)\underbrace{(-\eta \nabla L)} + \underbrace{\alpha \bar{v}}_{\to 0 \text{ when } \alpha = 0}$$

$$\bar{\beta} \leftarrow \bar{\beta} + \bar{v}$$

when $\alpha = 0$, Momentum $\longrightarrow$ GD

when $\alpha = 1$ $\longrightarrow$ X

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when $\alpha = 0$, Momentum $\longrightarrow$ GD

when $\alpha = 1$ $\longrightarrow$ X

$\alpha \approx 0.9$

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Note

$\alpha = 0$

$$\bar{v} \leftarrow (1-\alpha)\underbrace{(-\eta \nabla L)} + \underbrace{\alpha \bar{v}}_{0 \text{ when } \alpha=0}$$

$$\bar{\beta} \leftarrow \bar{\beta} + \bar{v}$$

when $\alpha=0$, Momentum $\longrightarrow$ GD

when $\alpha=1$ $\longrightarrow$ X

$\alpha \approx 0.9 \leftarrow$ pro

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Benefits

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Smoothing

$$v \leftarrow (1-\alpha)(-\eta \nabla) + \alpha v$$

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Benefits

Smoothing

$$v \leftarrow (1-\alpha)(-\eta \nabla) + \alpha v$$

smoothening

EWA

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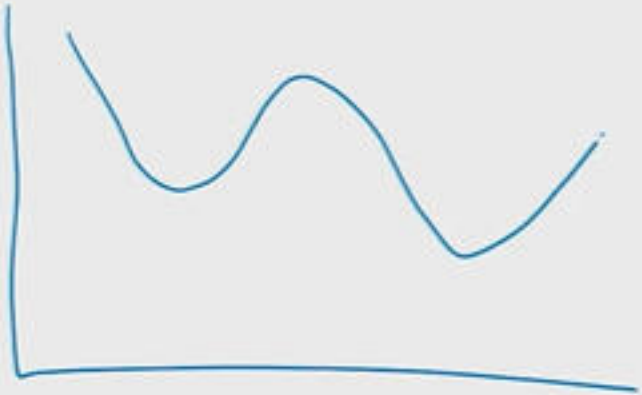
Benefits

Escapes local minima



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Benefits

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Escapes local minima

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Benefits

Escapes local minima

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Benefits

Escapes local minima

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Downsides

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Extra meta-parameter

α

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Downsides

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Extra meta-parameter

α

hyperparameter

→ Cross-validati

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Downsides

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Oscillations

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Downsides

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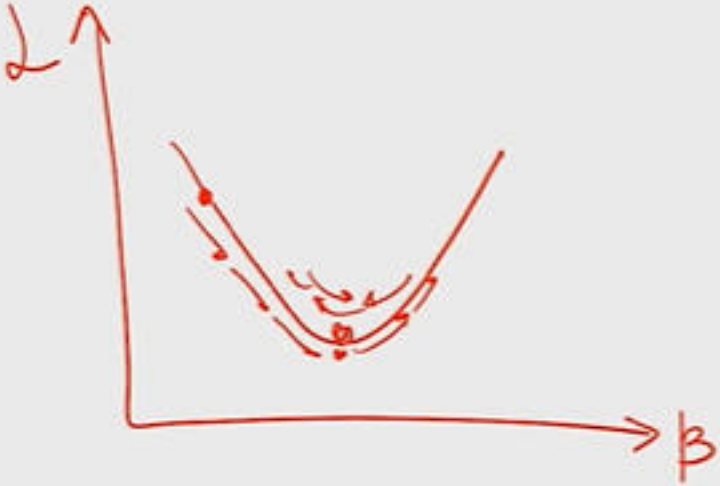
Oscillations



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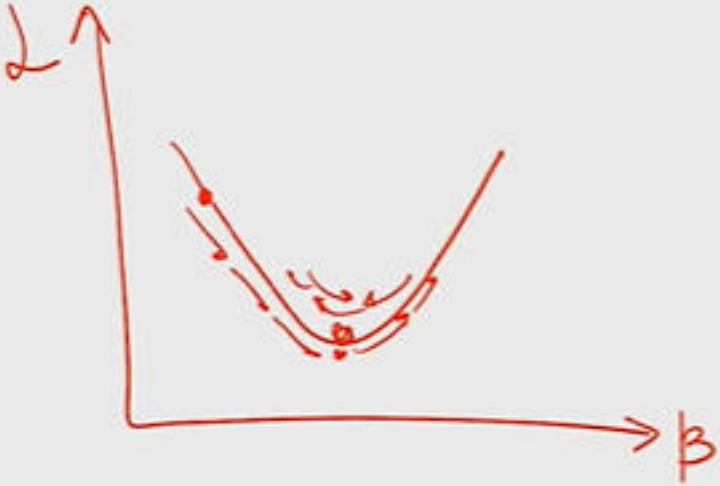
Downsides

Oscillations



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AdaGrad

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Topics

- The Expression
- Benefits
- Downsides

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AdaGrad

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Attempts to adapt the **step size**
to make them all **of the same scale**

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AdaGrad

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Attempts to adapt the **step size**
to make them all **of the same scale**

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The Expression

$$\beta \leftarrow \beta + \eta \frac{\partial \mathcal{L}}{\partial \beta}$$

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The Expression

$$\beta \leftarrow \beta + \eta \frac{\partial \mathcal{L}}{\partial \beta}$$

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The Expression

$$\beta_i \leftarrow \beta_i + \eta \frac{\partial L}{\partial \beta_i} \longleftarrow \text{ADAGRA}$$

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The Expression

$$\beta_i \leftarrow \beta_i + \eta \frac{\partial L}{\partial \beta_i} \longleftarrow \text{ADAGRAD}$$

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The Expression

$$\beta_i \leftarrow \beta_i + \frac{\eta}{\sqrt{c + \frac{\partial \mathcal{L}}{\partial \beta_i}}} \frac{\partial \mathcal{L}}{\partial \beta_i} \longleftarrow \text{ADAGRAD.}$$

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The Expression

$$\beta_i \leftarrow \beta_i + \frac{\eta}{\sqrt{c + \left(\frac{\partial L}{\partial \beta_i}\right)^2}} \frac{\partial L}{\partial \beta_i} \longleftarrow \text{ADAGRAD.}$$

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The Expression

$$\beta_i \leftarrow \beta_i + \frac{\eta}{\sqrt{c + \sum_t \left(\frac{\partial \mathcal{L}}{\partial \beta_i}\right)^2}} \frac{\partial \mathcal{L}}{\partial \beta_i} \longleftarrow \text{ADAGRAD.}$$

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The Expression

$$\beta_i \leftarrow \beta_i + \frac{\eta}{\sqrt{c + \sum_t \left(\frac{\partial L}{\partial \beta_i}\right)^2}} \frac{\partial L}{\partial \beta_i} \longleftarrow \text{ADAGRAD.}$$

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The Expression

$$\beta_i \leftarrow \beta_i + \frac{\eta}{\sqrt{c + \sum_{t'} \left(\frac{\partial \mathcal{L}}{\partial \beta_i}\right)^2}} \frac{\partial \mathcal{L}}{\partial \beta_i} \longleftarrow \text{ADAGRAD.}$$

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The Expression

$$\beta_i \leftarrow \beta_i + \frac{\eta}{\sqrt{c + \sum_{t=} \left(\frac{\partial L}{\partial \beta_i}\right)^2}} \underline{\frac{\partial L}{\partial \beta_i}} \longleftarrow \text{ADAGRAD.}$$

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The Expression

$$\beta_i \leftarrow \beta_i + \frac{\eta}{\sqrt{c + \sum_{t=1}^{s} \left(\frac{\partial L}{\partial \beta_i}\right)^2}} \frac{\partial L}{\partial \beta_i} \longleftarrow \text{ADAGRAD.}$$

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The Expression

$$\beta_i \leftarrow \beta_i + \frac{\eta}{\sqrt{c + \sum_{t=1}^{s} \left(\frac{\partial L}{\partial \beta_i}\right)^2}} \frac{\partial L}{\partial \beta_i} \longleftarrow \text{ADAGRAD.}$$

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The Expression

$$\beta_i \leftarrow \beta_i^{(s)} + \frac{\eta}{\sqrt{c + \sum_{t=1}^{s} \left(\frac{\partial \mathcal{L}}{\partial \beta_i}\right)^2}} \frac{\partial \mathcal{L}}{\partial \beta_i} \longleftarrow \text{ADAGRAD.}$$

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The Expression

$$\beta_i^{(s+1)} \longleftarrow \beta_i^{(s)} + \frac{\eta}{\sqrt{c + \sum_{t=1}^{s} \left(\frac{\partial \mathcal{L}}{\partial \beta_i}\right)^2}} \underline{\frac{\partial \mathcal{L}}{\partial \beta_i}} \longleftarrow \text{ADAGRAD.}$$

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The Expression

$$\beta_i^{(s+1)} \longleftarrow \beta_i^{(s)} + \frac{\eta}{\sqrt{c + \sum_{t=1}^{s} \left(\frac{\partial \mathcal{L}}{\partial \beta_i^{(s)}}\right)^2}} \underline{\frac{\partial \mathcal{L}}{\partial \beta_i^{(s)}}} \longleftarrow \text{ADAGRAD.}$$

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Benefits

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Not sensitive to meta-parameters

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Benefits

aws training and certification

Not sensitive to meta-parameters

η, c

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Benefits

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Very simple to implement

$$\frac{\partial}{\partial \beta_i^{(t)}}$$

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Benefits

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Very simple to implement

$$\left(\frac{\partial \mathcal{L}}{\partial \beta_i^{(t)}}\right) \quad \forall i, t.$$

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Downsides

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Learning rate death

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Downsides

Learning rate death

$$\frac{\eta}{\sqrt{c + \sum_{t=0}^{S} \left(\frac{\partial L}{\partial \beta_i^{(t)}} \right)^2}}$$

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Downsides

Learning rate death

$$\frac{1}{\sqrt{c + \sum_{t=0}^{S} \left(\frac{\partial L}{\partial \beta_i^{(t)}} \right)^2}}$$

large value. ⇒ learning rate becomes very s.

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Downsides

Learning rate death

$$\frac{1}{\sqrt{c + \sum_{t=0}^{S} \left(\frac{\partial L}{\partial \beta_i^{(t)}} \right)^2}}$$

large value. $\Rightarrow$ learning rate becomes very small

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Optimization

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Optimization is equal parts

art

and

science

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Optimization

Which method will work best depends on your data, and the only way to really know for sure is to **try** them out and select the method that produces the **best test loss**.

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Optimization

Honestly, many machine learning practitioners just pick a favorite.

For example, some practitioners like the comfort of a large body of literature with SGD.

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Discussion of Methods

For a robust discussion of possible methods, see:
http://ruder.io/optimizing-gradient-descent/

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Images

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- https://thenounproject.com/search/?q=science&i=1445239
- https://thenounproject.com/search/?q=pitfall&i=1189524
- https://thenounproject.com/search/?q=try%20again&i=451520
- https://thenounproject.com/search/?q=art&i=225590

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Regression for Machine Learning: In Summary

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Regression for Machine Learning: In Summary

Learning Outcomes

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In this track, you learnt how to:

- Describe how loss functions of regression models are motivated.
- Derive maximum likelihood estimators of simple statistical models.
- Adapt loss functions of regression models for problem-specific requirements including regularization.
- Understand batch, stochastic gradient training algorithms of regression models.
- Identify practical tricks for using training algorithms, such as momentum, Adagrad.

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Optional Reading

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- K. Murphy, Machine Learning: A Probabilistic Perspective
- C. Bishop, Pattern Recognition and Machine Learning
- T. Hastie, R. Tibshirani, J. Friedman, The Elements of Statistical Learning: Data Mining, Inference, and Prediction (available free online)

-0:14

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Knowledge Check: Regression - Course 5

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What is the Newton's method update step for OLS?

a. $\vec{\beta} - \frac{\eta}{N} X^T(\vec{y} - X\vec{\beta})$

b. $\vec{\beta} + (X^T X)^{-1} X^T \vec{y}$

c. $(X^T X)^{-1} X^T \vec{y}$

d. $\vec{\beta} + \frac{\eta}{N} X^T(\vec{y} - X\vec{\beta})$

Knowledge Check: Regression - Course 5

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What is the preferred ordering of data points for Stochastic Gradient Descent (SGD)?

a. Cycle through starting with the first element
b. Random selection
c. Shuffle and then cycle through
d. Cycle through starting with a random element

Knowledge Check: Regression - Course 5

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Which of the following is NOT an advantage of SGD over Gradient Descent?

a. SGD can be used with streaming data

b. SGD has lower computational complexity for large datasets

c. SGD requires fewer updates steps to converge (up to a small ϵ error)

d. SGD update step has lower memory requirements

Knowledge Check: Regression - Course 5

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Which of the following is a feature of Gradient Descent with Momentum? (choose all that apply)

a. It is a exponentially weighted average function of gradients computed at different coefficient values

b. It uses a single data point in each update step

c. It helps in avoiding convergence to local minima

d. Step size in a momentum update step is variable

Knowledge Check: Regression - Course 4

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Which of the following is the cost function $J(\beta)$ for logistic regression?

a. $\sum_{i=1}^{N} y_i \log\left(1 + e^{\beta^T x_i}\right) + (1 - y_i) \log\left(1 + e^{\beta^T x_i}\right)$

b. $\sum_{i=1}^{N} y_i \log\left(1 + e^{-\beta^T x_i}\right) + (1 - y_i) \log\left(1 + e^{-\beta^T x_i}\right)$

c. $\sum_{i=1}^{N} y_i \log\left(1 + e^{\beta^T x_i}\right) + (1 - y_i) \log\left(1 + e^{-\beta^T x_i}\right)$

d. $\sum_{i=1}^{N} y_i \log\left(1 + e^{-\beta^T x_i}\right) + (1 - y_i) \log\left(1 + e^{\beta^T x_i}\right)$

$$J(\beta) = -\sum_{i=1}^{N} \left[y_i \log\left(\phi(\bar{x}_i \cdot \bar{\beta})\right) + (1 - y_i) \log\left(1 - \phi(\bar{x}_i \cdot \bar{\beta})\right) \right]$$

$$\phi(x) = \frac{1}{1 + e^{-x}}$$

Knowledge Check: Regression - Course 4

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Which of the following is the gradient of $J(\beta)$ in matrix form?

a. $-X^T(\vec{y} - \Phi\left(X\vec{\beta}\right))$

b. $-(\vec{y} - \Phi\left(X\vec{\beta}\right))X^T$

c. $-(\vec{y} - \Phi\left(X\vec{\beta}\right))$

d. $-X^T(\vec{y} - \Phi\left(X\vec{\beta}\right))X^T$

Knowledge Check: Regression - Course 4

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Write down the update step for $J(\beta)$ with Gradient Descent?

a. $\vec{\beta} - \frac{\eta}{N} X^T (\vec{y} + \Phi\left(X\vec{\beta}\right))$

b. $\vec{\beta} - \frac{\eta}{N} X^T (\vec{y} - \Phi\left(X\vec{\beta}\right))$

c. $\vec{\beta} + \frac{\eta}{N} X^T (\vec{y} - \Phi\left(X\vec{\beta}\right))$

d. $\vec{\beta} + \eta X^T (\vec{y} + \Phi\left(X\vec{\beta}\right))$

Knowledge Check: Regression - Course 4

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Write down the update step for $J(\beta)$ with Gradient Descent?

a. $\vec{\beta} - \frac{\eta}{N} X^T(\vec{y} + \Phi\left(X\vec{\beta}\right))$

b. $\vec{\beta} - \frac{\eta}{N} X^T(\vec{y} - \Phi\left(X\vec{\beta}\right))$

c. $\vec{\beta} + \frac{\eta}{N} X^T(\vec{y} - \Phi\left(X\vec{\beta}\right))$

d. $\vec{\beta} + \eta X^T(\vec{y} + \Phi\left(X\vec{\beta}\right))$

$$\vec{\beta} \leftarrow \vec{\beta} + \frac{\eta}{N}\left(-\frac{\partial J}{\partial \vec{\beta}}\right)$$

$$= \vec{\beta} + \frac{\eta}{N} X^T\left(\vec{y} - \Phi\left(X\vec{\beta}\right)\right)$$

Knowledge Check: Regression - Course 3

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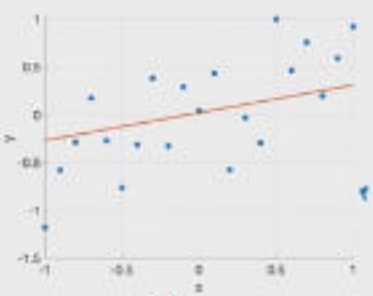
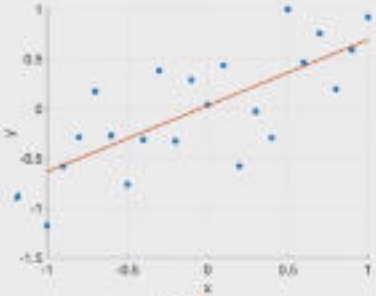
Assign each figure below to the appropriate model. Assume that δ^2 is the hyperparameter for L2 regularization and λ as the hyperparameter for radial basis function (RBFs): $K(x, \mu_i, \lambda) = e^{-\left(\frac{1}{\lambda}\right)\|x - \mu_i\|^2}$

a. Linear regression δ2=0.01
b. Linear regression δ2=10
c. Linear regression with RBFs as features δ2=0.01 and λ=1
d. Linear regression with RBFs as features δ2=10 and λ=1



(b)



(a)

Knowledge Check: Regression - Course 3

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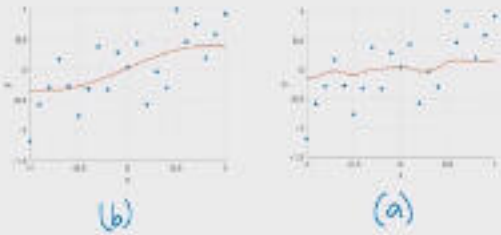
Assign each figure below to the appropriate model. Assume that δ^2 is the hyperparameter for L2 regularization and λ as the hyperparameter for radial basis function (RBFs): $K(x, \mu_i, \lambda) = e^{-\left(\frac{1}{\lambda}\right)\|x - \mu_i\|^2}$

a. Linear regression with RBFs as features δ2=10 and λ=0.01
b. Linear regression with RBFs as features δ2=10 and λ=1
c. Linear regression δ2=0.01
d. Linear regression δ2=10



Knowledge Check: Regression - Course 3

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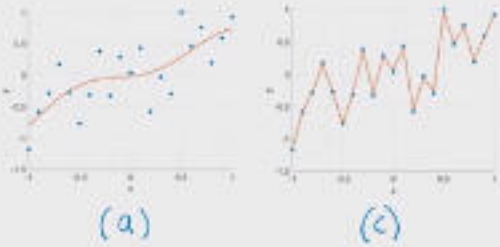
a. Linear regression with RBFs as features δ2=0.01 and λ=1
b. Linear regression δ2=0.01
c. Linear regression with RBFs as features δ2=0.01 and λ=0.01
d. Linear regression δ2=10



Knowledge Check: Regression - Course 2

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Suppose I tossed a coin 5 times and observed the outcome: (T H T T H). The coin outcome follows a Bernoulli distribution. The Bernoulli distribution has a single parameter, 'p', which represents the probability of seeing a Head. What is the maximum likelihood estimate of p?

a. 1/6

b. 3/5

c. 2/5

d. 5/6

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$$L = P(T)P(H)P(T)P(T)P(H) \quad \left(= P(\{T, H, T, T, H\})\right)$$

$$= (1-p)(p)(1-p)(1-p)(p)$$

$$= p^2(1-p)^3$$

$$\log L = 2\log(p) + 3\log(1-p)$$

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$$\frac{d(\log L)}{dp} = 0 \Rightarrow \frac{2}{p} + \frac{3}{1-p}(-1) = 0$$

$$\Rightarrow p =$$

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Now, $J(\beta) = \sum_{i=1}^{N} \omega_i \left(y_i - \vec{x_i} \cdot \vec{\beta}\right)^2 = \left(\vec{y} - X\vec{\beta}\right)^T W(\vec{y} - X\vec{\beta})$

What does the expression $\frac{\partial J}{\partial \beta}$ evaluate to?

$$\frac{\partial J}{\partial \beta} = \frac{\partial}{\partial \vec{\beta}}\left(\vec{y}^T - \vec{\beta}^T X^T\right)\left(W\vec{y} - WX\vec{\beta}\right)$$

$$= \frac{\partial}{\partial \vec{\beta}}\left[\vec{y}^T W\vec{y} - \vec{\beta}^T X^T W\vec{y} + \vec{\beta}^T X^T W X\vec{\beta} - \vec{y}^T W X\vec{\beta}\right]$$

a. $-2X^T\vec{y} + 2X^TX\vec{\beta}$

b. $-X^TW\vec{y} + X^TWX\vec{\beta}$

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$$= -X^T W^T \vec{y}$$

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Knowledge Check: Regression - Course 1

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Given the following three data points, please calculate (by hand) the closed form solution for linear regression and predict the value of y when x = 2

a. $Y = -0.5x + 0.3$

b. $Y = 0.5x + 0.3$

c. $Y = 0.5x - 0.3$

d. $Y = -0.5x - 0.3$

x	y
-1	0.8
0	0.3
1	-0.2

Knowledge Check: Regression - Course 1

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x	y
-1	0.8
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1	-0.2

$\bar{x} = 0$

$\bar{y} = \frac{0.8 + 0.3 - 0.2}{3}$

$= 0.3$

$\boxed{\hat{y} = ax + b}$

$a = \frac{Cov(X,Y)}{var(X)}$

$= \frac{(-1-0)(0.8-0.3) + 0 + (1-0)(-0.2-0.3)}{1^2 + 0^2 + 1^2}$

$= -1/2$

$b = \bar{y} - a\bar{x}$

$= 0.3 - (-1/2)(0)$

$= 0.3$

Knowledge Check: Regression - Course 1

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Which one of the following is a linear function?

a. $y = 0.2x_1 + 2.0$

b. $y = \sin(0.2x_1 + 2.0)$

c. $y = 2x_1^2 + 5z_2^2$

d. $y = \log(x_1 + x_2)$

e. $y = \sin(x_1) - \cos(x_2)$

Knowledge Check: Regression - Course 1

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Does high R^2 always imply a good fit?

a. True

b. False

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Certificate of Completion

Hem Bahadur Gurung

Has successfully completed

Linear and Logistic Regression

Director, Training and Certification	8 1/2 hours	10 September, 2021
	Duration	Completion Date