CS 6316 Machine Learning

Review of Linear Algebra and Probability

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Overview

- 1. Course Information
- 2. Basic Linear Algebra
- 3. Probability Theory
- 4. Expectation
- 5. Statistical Estimation

Course Information

Instructors

- Yangfeng Ji
 - ► Office hour: Wednesday 11 AM 12 PM
 - Office: Rice 510
- ► Hanjie Chen (TA)
 - ► Office hour: Tuesday and Thursday 1 PM 2 PM
 - Office: Rice 442

Goal

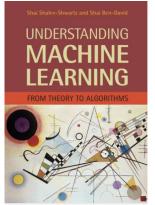
Understand the basic concepts and models from the computational perspective

To

- provide a wide coverage of basic topics in machine learning
- discuss a few fundamental concepts in each topic

Textbook

Shalev-Shwartz and Ben-David. *Understanding Machine Learning: From Theory to Algorithms*. 2014¹



//www.cse.huji.ac.il/~shais/UnderstandingMachineLearning/index.html

¹https:

Outline

This course will cover the basic materials on the following topics

- 1. Learning theory
- 2. Linear classification and regression
- 3. Model selection and validation
- 4. Boosting and support vector machines
- 5. Neural networks
- 6. Clustering and dimensionality reduction

Outline (II)

The following topics will not be the emphasis of this course

- Statistical modeling
 - Statistical Learning and Graphical Models by Farzad Hassanzadeh
- ▶ Deep learning
 - Deep Learning for Visual Recognition by Vicente Ordonez-Roman

Reference Courses

For fans of machine learning:

- ▶ Shalev-Shwartz. Understanding Machine Learning. 2014
- ▶ Mohri. Foundations of Machine Learning. Fall 2018

Reference Books

For fans of machine learning:

- ► Hastie, Tibshirani, and Friedman. The Elements of Statistical Learning (2nd Edition). 2009
- Murphy. Machine Learning: A Probabilistic Perspective.
 2012
- ▶ Bishop. Pattern Recognition and Machine Learning. 2006
- Mohri, Rostamizadeh, and Talwalkar. Foundations of Machine Learning. 2nd Edition. 2018

Homework and Grading Policy

- ► Homeworks (75%)
 - ► Five homeworks, each of them worth 15%
- ► Final project (22%)
 - Project proposal: 5%
 - ► Midterm report: 5%
 - ► Final project presentation: 6%
 - Final project report: 6%
- ► Class attendance (3%): we will take attendance at three randomly-selected lectures. Each is worth 1%

Grading Policy

The final grade is threshold-based instead of percentage-based

Point range	Letter grade
[99 100]	A+
[94 99)	Α
[90 94)	Α-
[88 90)	B+
[83 88)	В
[80 83)	B-
[74 80)	C+
[67 74)	С
[60 67)	C-

Late Penalty

- Homework submission will be accepted up to 72 hours late, with 20% deduction per 24 hours on the points as a penalty
- ► It is usually better if students just turn in what they have in time
- ▶ Submission will not be accepted if more than 72 hours late
- Do not submit the wrong homework late penalty will be applied if resubmit after deadline

Violation of the Honor Code

Plagiarism, examples are

- in a homework submission, copying answers from others directly (even, with some minor changes)
- in a report, copying texts from a published paper (even, with some minor changes)
- in a code, using someone else's functions/implementations without acknowledging the contribution

Course Webpage

http://yangfengji.net/uva-ml-course/

which contains all the information you need about this course.

Basic Linear Algebra

Linear Equations

Consider the following system of equations

$$4x_1 - 5x_2 = -13$$

$$-2x_1 + 3x_2 = 9$$
(1)

In matrix notation, it can be written as a more compact from

$$\mathbf{A}x = b \tag{2}$$

with

$$\mathbf{A} = \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix} \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} -13 \\ 9 \end{bmatrix} \tag{3}$$

Basic Notation

$$\mathbf{A} = \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix} \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} -13 \\ 9 \end{bmatrix}$$

- ▶ $A \in \mathbb{R}^{m \times n}$: a matrix with *m* rows and *n* columns
 - ▶ The element on the *i*-th row and the *j*-th column is denoted as $a_{i,j}$
- ▶ $x \in \mathbb{R}^n$: a vector with n entries. By convention, an n-dimensional vector is often thought of as matrix with n rows and 1 column, known as a column vector.
 - ▶ The *i*-th element is denoted as x_i

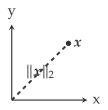
Vector Norms

- A norm of a vector ||x|| is informally a measure of the "length" of the vector.
- ► Formally, a norm is any function $f : \mathbb{R}^n \to \mathbb{R}$ that satisfies four properties
 - 1. $f(x) \ge 0$ for any $x \in \mathbb{R}^n$
 - 2. f(x) = 0 if and only if x = 0
 - 3. $f(ax) = |a| \cdot f(x)$ for any $x \in \mathbb{R}^n$
 - 4. $f(x + y) \le f(x) + f(y)$, for any $x, y \in \mathbb{R}^n$

ℓ_2 Norm

The ℓ_2 norm of a vector x is defined as

$$||x||_2 = \sqrt{\sum_{i=1}^n x_i^2} \tag{4}$$



Exercise: prove ℓ_1 norm satisfies all four properties

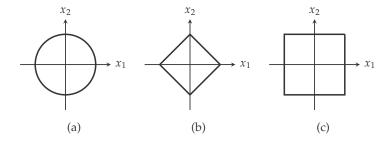
ℓ_1 Norms

 ℓ_1 norm is defined as

$$||x||_1 = \sum_{i=1}^n |x_i| \tag{5}$$

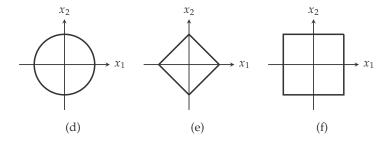
Quiz

For a two-dimensional vector $x = [x_1, x_2]$, which of the following plot is $||x||_1 = 1$?



Quiz

For a two-dimensional vector $x = [x_1, x_2]$, which of the following plot is $||x||_1 = 1$? Answer: (b)



Dot Product

The dot product of x, $y \in \mathbb{R}^n$ is defined as

$$\langle x, y \rangle = x^{\mathsf{T}} y = \sum_{i=1}^{n} x_i y_i$$
 (6)

where x^{T} is the transpose of x.

Some special cases

- Example: if x = (0, 0, ..., 1, ..., 0), then $\langle x, y \rangle = y_i$
- More general, if x is an unit vector ($||x||_2 = 1$), then $\langle x, y \rangle$ is the projection of y on the direction of x



Cauchy-Schwarz Inequality

For all $x, y \in \mathbb{R}^n$

$$|\langle x, y \rangle| \le ||x||_2 ||y||_2 \tag{7}$$

with equality if and only if $x = \alpha y$ with $\alpha \in \mathbb{R}$

Proof:

Let $\tilde{x} = \frac{x}{\|x\|_2}$ and $\tilde{y} = \frac{y}{\|y\|_2}$, then \tilde{x} and \tilde{y} are both unit vectors.

Based on the geometric interpretation on the previous slide, we have

$$\langle \tilde{x}, \tilde{y} \rangle \le 1$$
 (8)

if and only if $\tilde{x} = \tilde{y}$.

Frobenius Norm

The Forbenius norm of a matrix $\mathbf{A} = [a_{i,j}] \in \mathbb{R}^{m \times n}$ denoted by $\|\cdot\|_F$ is defined as

$$\|\mathbf{A}\|_F = \left(\sum_{i} \sum_{j} a_{i,j}^2\right)^{1/2} \tag{9}$$

▶ The Frobenius norm can be interpreted as the ℓ_2 norm of a vector when treating **A** as a vector of size mn.

Two Special Matrices

▶ The identity matrix, denoted as $\mathbf{I} \in \mathbb{R}^{n \times n}$], is a square matrix with ones on the diagonal and zeros everywhere else.

$$\mathbf{I} = \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} \tag{10}$$

A diagonal matrix, denoted as $\mathbf{D} = \operatorname{diag}(d_1, d_2, \dots, d_n)$, is a matrix where all non-diagonal elements are o.

$$\mathbf{D} = \begin{bmatrix} d_1 & & & \\ & \ddots & & \\ & & d_n \end{bmatrix} \tag{11}$$

Inverse

The *inverse* of a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is denoted as \mathbf{A}^{-1} , which is the unique matrix such that

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{I} = \mathbf{A}\mathbf{A}^{-1} \tag{12}$$

- Non-square matrices do not have inverses (by definition)
- Not all square matrices are invertible
- ► The solution of the linear equations in Eq. (1) is $x = A^{-1}b$

Orthogonal Matrices

► Two vectors $x, y \in \mathbb{R}^n$ are orthogonal if $\langle x, y \rangle = 0$



A square matrix $\mathbf{U} \in \mathbb{R}^{n \times n}$ is orthogonal, if all its columns are orthogonal to each other *and* normalized (orthonormal)

$$\langle u_i, u_j \rangle = 0, ||u_i|| = 1, ||u_j|| = 1$$
 (13)

for $i, j \in [1, n]$ and $i \neq j$

Furthermore, $\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{I} = \mathbf{U}\mathbf{U}^{\mathsf{T}}$, which further implies $\mathbf{U}^{-1} = \mathbf{U}^{\mathsf{T}}$

Symmetric Matrices

A symmetric matrix is defined as

$$\mathbf{A}^{\mathsf{T}} = \mathbf{A} \tag{14}$$

or, in other words,

$$a_{i,j} = a_{j,i} \tag{15}$$

Comments

- ▶ The identity matrix **I** is symmetric
- A diagonal matrix is symmetric

Eigen Decomposition

Every symmetric matrix **A** can be decomposed as

$$\mathbf{A} = \mathbf{U}\Lambda\mathbf{U}^{\mathsf{T}} \tag{16}$$

with

- ▶ **Q** is an orthogonal matrix (Slide 27)
- Exercise: Show $\mathbf{A}^{-1} = \mathbf{U}\Lambda^{-1}\mathbf{U}^{\mathsf{T}}$ with $\Lambda^{-1} = \mathrm{diag}(\frac{1}{\lambda_1}, \dots, \frac{1}{\lambda_n})$

Symmetric Positive Semidefinite Matrices

A symmetric matrix $\mathbf{P} \in \mathbb{R}^{n \times n}$ is positive semidefinite if and only if

$$x^{\mathsf{T}} \mathbf{P} x \ge 0 \tag{17}$$

for all $x \in \mathbb{R}^n$.

Symmetric Positive Semidefinite Matrices

A symmetric matrix $\mathbf{P} \in \mathbb{R}^{n \times n}$ is positive semidefinite if and only if

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for all $x \in \mathbb{R}^n$.

Eigen decomposition (Slide 29) of P as

$$\mathbf{P} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{\mathsf{T}} \tag{18}$$

with $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ and

$$\lambda_i \ge 0 \tag{19}$$

Symmetric Positive Definite Matrices

A symmetric matrix $\mathbf{P} \in \mathbb{R}^{n \times n}$ is positive definite if and only if

$$x^{\mathsf{T}} \mathbf{P} x > 0 \tag{20}$$

for all $x \in \mathbb{R}^n$.

► Eigen values of **P**, $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$ with

$$\lambda_i > 0 \tag{21}$$

Exercise: if you one of the eigen values $\lambda_i < 0$, show that you can also find a vector x such that $x^T P x < 0$

Quiz

The identity matrix I is

- a diagonal matrix?
- a symmetric matrix?
- an orthogonal matrix?
- a positive (semi-)definite matrix?

Further reference [Kolter and Do, 2015]

Quiz

The identity matrix I is

- ▶ a diagonal matrix? ✓
- ▶ a symmetric matrix? ✓
- ▶ an orthogonal matrix? ✓
- ▶ a positive (semi-)definite matrix? ✓

Further reference [Kolter and Do, 2015]

Probability Theory

What is Probability?



The probability of landing heads is 0.52

Two interpretations

Frequentist Probability represents the *long-run frequency* of an event

► If we flip the coin many times, we expect it to land heads about 52% times

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Frequentist Probability represents the *long-run frequency* of an event

► If we flip the coin many times, we expect it to land heads about 52% times

Bayesian Probability quantifies our *(un)certainty* about an event

► We believe the coin is 52% of chance to land head on the next toss

Bayesian Interpretation

Example scenarios of Bayesian interpretation of probability:





Binary Random Variables

- **Event** *X*. Such as
 - the coin will lead head on the next toss
 - it will rain tomorrow
- ▶ Sample space of $X \in \{\text{false, true}\}\ \text{or for simplicity}\ \{0, 1\}$
- ▶ Probability P(X = x) or P(x)
- ► Let *X* be the event that *the coin will lead head on the next toss*, then the probability from the previous example is

$$P(X=1) = 0.52 \tag{22}$$

Bernoulli Distribution

Given the binary random variable X and its sample space as $\{0,1\}$

$$P(X = x) = \theta^{x} (1 - \theta)^{1 - x}$$

with a single parameter θ as

$$\theta = P(X=1)$$



Jacob Bernoulli

- Let *X* be the number of heads
- ► Sample space of $X \in \{0, 1, 2\}$

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- ► Assume we use the same coin, the probability distribution of *X*
 - $P(X = 0) = (1 \theta)^2$

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 - $P(X = 0) = (1 \theta)^2$
 - ► $P(X = 2) = \theta^2$

- Let *X* be the number of heads
- ► Sample space of $X \in \{0, 1, 2\}$
- Assume we use the same coin, the probability distribution of *X*
 - $P(X = 0) = (1 \theta)^2$
 - ► $P(X = 2) = \theta^2$
 - $P(X = 1) = \theta(1 \theta) + (1 \theta)\theta = 2\theta(1 \theta)$

General Case: Binomial Distribution

Consider a general case, in which we toss the coin n times, then the random variable Y can be formulated as a binomial distribution

$$P(Y = k) = \binom{n}{k} \theta^k (1 - \theta)^{n-k}$$
 (23)

where

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

is the binomial coefficient and

$$n! = n \cdot (n-1) \cdot (n-2) \cdots 1$$

Tossing a Dice



How to define the corresponding random variable?

- $X \in \{1, 2, 3, 4, 5, 6\}$
- $X \in \{100000, 010000, 001000, 000100, 000010, 000001\}$

Categorical Distribution

$$P(X = x) = \prod_{k=1}^{6} (\theta_k)^{x_k}$$
 (24)

where

- $x = (x_1, x_2, \dots, x_6)$
- ► $x_k \in \{0, 1\}$, and
- $\{\theta_k\}_{k=1}^6$ are the parameters of this distribution, which is also the probability of side k showing up.

Multinomial Distribution

Repeat the previous event n times, the corresponding probability distribution is modeled as

$$P(X = x) = \binom{n}{x_1 \cdots x_K} \prod_{k=1}^K \theta_k^{x_k}$$
 (25)

where $x_k \in \{0, 1, 2, ..., n\}$ with

$$\sum_{k=1}^{K} x_k = n$$

and

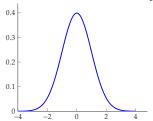
$$\binom{n}{x_1\cdots x_K} = \frac{n!}{x_1!\cdots x_K!}$$

Gaussian Distribution

A random variable $X \in \mathbb{R}$ is said to follow a normal (or Gaussian) distribution $\mathcal{N}(\mu, \sigma^2)$ if its probability density function is given by

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2}\right)$$
 (26)

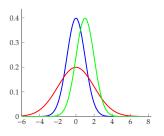
- μ: mean
- $ightharpoonup \sigma^2$: variance
- ▶ Probability of $X \in [a, b]$: $P(a \le X \le b) = \int_a^b f(x) dx$



Gaussian Distribution (II)

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2}\right)$$
 (27)

There examples of Gaussian distributions



- **Blue**: $\mathcal{N}(0,1)$ (standard normal distribution)
- ▶ Red: $\mathcal{N}(0,2)$
- ▶ Green: $\mathcal{N}(1,1)$

Probability of Two Random Variables

Modeling two random variables together with a **joint** distribution

$$P(X \cap Y) \tag{28}$$

Related concepts

- ► Independence
- Conditional probability and chain rule
- ► Bayes' rule

Independence

$$P(X \cap Y) = P(X) \cdot P(Y)$$
 (29)

where

$$P(X) = \sum_{Y} P(X \cap Y) (30)$$

$$P(Y) = \sum_{X} P(X \cap Y) (31)$$

are two marginal distributions.

Independence

$$P(X \cap Y) = P(X) \cdot P(Y)$$
 (29)

where

$$P(X) = \sum_{Y} P(X \cap Y) (30)$$

$$P(Y) = \sum_{X} P(X \cap Y) (31)$$

are two marginal distributions.

- ► *X*: whether it is cloudy
- Υ: whether it will rain

$P(X\cap Y)$	X = 0	X = 1
Y = 0	0.35	0.15
Y = 1	0.05	0.45

Conditional Probability

Conditional probability of *Y* given *X*

$$P(Y \mid X) = \frac{P(X \cap Y)}{P(X)} \tag{32}$$

Example: document classification

- ► X: a document
- Y: the label of this document

Conditional Probability

- ➤ *X*: whether it is cloudy
- Y: whether it will rain

$P(X\cap Y)$	X = 0	X = 1
Y = 0	0.35	0.15
Y = 1	0.05	0.45

- ▶ $P(Y \mid X = 1)$:
 - $P(Y = 0 \mid X = 1) = 0.25,$
 - $P(Y = 1 \mid X = 1) = 0.75$

Conditional Probability

- X: whether it is cloudy
- Y: whether it will rain

$P(X\cap Y)$	X = 0	X = 1
Y = 0	0.35	0.15
Y = 1	0.05	0.45

- ▶ $P(Y \mid X = 1)$:
 - $P(Y = 0 \mid X = 1) = 0.25,$
 - $P(Y = 1 \mid X = 1) = 0.75$
- P(Y): P(Y = 0) = P(Y = 1) = 0.5

Multivariate Gaussian

The probability density function of a multivariate Gaussian distribution $\mathcal{N}(\mu, \Sigma)$ is defined as

$$f(x) = \frac{1}{(2\pi)^{n/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu)^{\mathsf{T}} \Sigma^{-1}(x-\mu)\right)$$
(33)

where

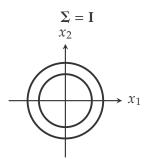
- \blacktriangleright μ is the *n*-dimensional mean vector and
- \triangleright Σ is the $n \times n$ covariance matrix.

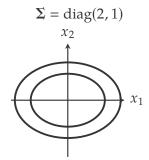
Covariance Matrix Σ

Assume $\mu = 0$, the probability density function is

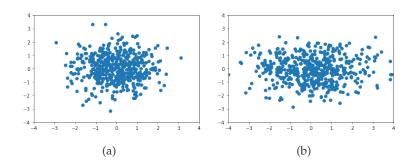
$$f(x) \propto \exp\left(-\frac{1}{2}x^{\mathsf{T}}\Sigma^{-1}x\right)$$
 (34)

In general, Σ is required to be a symmetric positive definite matrix





Sampling from Gaussians



- (a) : $\Sigma = I$
- (b) : $\Sigma = diag(2, 1)$

Exercise: Sample from an arbitrary Gaussian distribution

Sum Rule

Given two random variables X and Y, without any additional assumption we have

$$P(X \cup Y) = P(X) + P(Y) - P(X \cap Y) \tag{35}$$

► If *X* and *Y* are independent, then

$$P(X \cap Y) = 0 \quad \text{and} \quad P(X \cup Y) = P(X) + P(Y) \tag{36}$$

► *Exercise*: Prove the following inequality by generalizing the sum rule in

$$P(\cup_{i=1}^{n} X_i) \le \sum_{i=1}^{n} P(X_i)$$
(37)

This inequality is called the union bound.

Chain Rule

Any joint probability of two random variable can be decomposed as

$$P(X,Y) = P(X) \cdot P(Y \mid X) = P(Y) \cdot P(X \mid Y) \tag{38}$$

No independence assumption is needed

Chain Rule

Any joint probability of two random variable can be decomposed as

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No independence assumption is needed

The chain rule can be easily generalized

$$P(X_{1}, X_{2}, \cdots, X_{k}) = P(X_{1})P(X_{2}, \cdots, X_{k} \mid X_{1})$$

$$= P(X_{1})P(X_{2} \mid X_{1})P(X_{3}, \cdots, X_{k} \mid X_{2}, X_{1})$$

$$= P(X_{1})P(X_{2} \mid X_{1})P(X_{3} \mid X_{2}, X_{1}) \cdots$$

$$P(X_{k} \mid X_{1}, \cdots, X_{k-1})$$
(39)

Inverse Probability

Given

- \triangleright P(Y): prior probability, and
- \triangleright $P(X \mid Y)$: conditional probability of X given Y,

we can compute the probability $P(Y \mid X)$ using Bayes' rule as

$$P(Y \mid X) = \frac{P(Y)P(X \mid Y)}{P(X)} \tag{40}$$

where

$$P(X) = \sum_{Y} P(Y)P(X \mid Y) \tag{41}$$

Example: The burglar alarm

Two random variables, alarm A and burglar B

- ► $P(A = 1 \mid B = 1) = 0.99$: burglar happens, alarm rings
- ► $P(A = 1 \mid B = 0) = 0.001$: burglar does not happen, alarm rings
- ► P(B = 1) = 0.01: burglar rate

Question: if the alarm rang, what is the probability of a burglar happened?

$$P(B=1 \mid A=1) (42)$$

Example: The burglar alarm (II)

- $ightharpoonup P(A = 1 \mid B = 1) = 0.99$: burglar happens, alarm rings
- ► $P(A = 1 \mid B = 0) = 0.001$: burglar does not happen, alarm rings
- ► P(B = 1) = 0.01: burglar rate

Question: if the alarm rang, what is the probability of a burglar happened?

$$\begin{split} P(B=1 \mid & A=1) \\ &= \frac{P(B=1)P(A=1 \mid B=1)}{P(A=1 \mid B=1)P(B=1) + P(A=1 \mid B=0)P(B=0)} \\ &= \frac{0.01 \times 0.99}{(0.01 \times 0.99) + (0.001 \times (1-0.01))} \\ &\approx 0.91 \end{split}$$

Expectation

Expectation

The expectation or expected value of a function h(x) with respect to a probability distribution P(X) is defined as

$$E[h(x)] = \sum P(x)h(x) \tag{43}$$

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$$E[h(x)] = \sum_{x} P(x)h(x) \tag{43}$$

The number of ice creams [Eisenstein, 2018]

- ▶ If it is sunny, Lucia will eat three ice creams
- ▶ If it is rainy, she will eat only one ice cream
- ► There is a 80% chance it will be sunny

The expected number of ice creams she will eat is

$$0.8 \times 3 + 0.2 \times 1 = 2.6 \tag{44}$$

Mean

Let h(x) = x, the expectation is the mean value of the random variable X (discrete random variable)

$$E[X] = \sum_{x} x P(x) \tag{45}$$

or, (continuous random variable)

$$E[X] = \int_{x} x f(x) \tag{46}$$

A Bernoulli distribution P(X) with the parameter θ , $P(X = x) = \theta^x (1 - \theta)^{(1-x)}$

$$E[X] = 1 \cdot \theta + 0 \cdot (1 - \theta) = \theta \tag{47}$$

Variance

The variance of a random variable gives a measure of how much the values of this random variable vary

$$Var[X] = E[(X - E[X])^{2}]$$

$$= E[X^{2} - 2XE[X] + E[X]^{2}]$$

$$= E[X^{2}] - 2E[X]E[X] + E[X]^{2}$$

$$= E[X^{2}] - E[X]^{2}$$
(48)

Variance: Example

A Bernoulli distribution
$$P(X)$$
 with the parameter θ ,
$$P(X = x) = \theta^x (1 - \theta)^{(1-x)}$$

$$Var[X] = E[X^2] - E[X]^2 = p - p^2 \tag{49}$$

Exercise: Compute the mean and variance of a categorical distribution

Statistical Estimation

Statistics is, in a certain sense, the inverse of probability theory.

- ▶ Observed: values of random variables
- Unknown: the model
- ► Task: infer the model from the observed data

Likelihood-based Estimation

For a probability $P(X; \theta)$ with θ as the unknown parameter, likelihood-based estimation with observations $\{x^{(1)}, x^{(2)}, \dots, x^{(n)}\}$ requires two steps

- 1. Define a likelihood function with observations
- 2. Optimize the likelihood function to estimate θ

Likelihood Function

$$L(\theta) = \prod_{i=1}^{n} P(x^{(i)}; \theta)$$
 (50)

Alternatively, the corresponding log-likelihood function

$$\ell(\theta) = \log L(\theta)$$

$$= \sum_{i=1}^{n} \log P(x^{(i)}; \theta)$$
(51)

Maximum Likelihood Estimation

$$\hat{\theta} = \operatorname*{argmax} \ell(\theta) \tag{52}$$

Usually

$$\frac{\partial \ell(\theta)}{\partial \theta} = \sum_{i=1}^{n} \frac{\partial \log P(x^{(i)}; \theta)}{\partial \theta}$$
 (53)

Example: Bernoulli Distribution

Consider a Bernoulli distribution $P(X; \theta)$ with the parameter $\theta = P(X = 1; \theta)$ unknown

$$P(X = x; \theta) = \theta^{x} (1 - \theta)^{(1-x)}$$
(54)

Example: Bernoulli Distribution

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With *n* observations $\{x^{(1)}, x^{(2)}, \dots, x^{(n)}\}$, the likelihood function is

$$\ell(\theta) = \sum_{i=1}^{n} \log P(x^{(i)}; \theta)$$

$$= \sum_{i=1}^{n} \{x^{(i)} \log \theta + (1 - x^{(i)}) \log(1 - \theta)\}$$
 (55)

Example: Bernoulli Distribution (II)

The derivative with respect to θ

$$\frac{\partial \ell(\theta)}{\partial \theta} = \sum_{i=1}^{n} \left\{ \frac{x^{(i)}}{\theta} - \frac{1 - x^{(i)}}{1 - \theta} \right\} \tag{56}$$

Example: Bernoulli Distribution (II)

The derivative with respect to θ

$$\frac{\partial \ell(\theta)}{\partial \theta} = \sum_{i=1}^{n} \left\{ \frac{x^{(i)}}{\theta} - \frac{1 - x^{(i)}}{1 - \theta} \right\} \tag{56}$$

Let $\frac{\partial \ell(\theta)}{\partial \theta} = 0$, we have

$$\theta = \frac{\sum_{i=1}^{n} x^{(i)}}{n} \tag{57}$$

Example: Bernoulli Distribution (III)

Assume the n = 7 observations are

$$\{0, 1, 1, 0, 0, 1, 0\},\$$

then

$$\theta = \frac{3}{7} \tag{58}$$

Reference



Eisenstein, J. (2018).

Natural Language Processing.

MIT Press.



Kolter, Z. and Do, C. (2015). Linear algebra review and reference.