Mathematics for Machine Learning

— Probability & Distributions (Supplementary):

Sum Rule, Product Rule, Bayes' Theorem & Summary Statistics

Joseph Chuang-Chieh Lin

Department of Computer Science & Information Engineering,
Tamkang University

Fall 2023

Credits for the resource

- The slides are based on the textbooks:
  - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
  - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.*
- We could partially refer to the monograph:
  Francesco Orabona: A Modern Introduction to Online Learning. https://arxiv.org/abs/1912.13213

Outline

Outline

Sum Rule (1/2)

- $\mathbf{x}, \mathbf{y}$: random variables (vectors).
- $p(\mathbf{x}, \mathbf{y})$: joint distribution of $\mathbf{x}, \mathbf{y}$.
- $p(\mathbf{y} \mid \mathbf{x})$: conditional probability of $\mathbf{y}$ given $\mathbf{x}$.

Sum Rule

$$p(\mathbf{x}) = \begin{cases} \sum_{\mathbf{y} \in \mathcal{Y}} p(\mathbf{x}, \mathbf{y}) & \text{if } \mathbf{y} \text{ is discrete} \\ \int_{\mathcal{Y}} p(\mathbf{x}, \mathbf{y}) \mathrm{d}\mathbf{y} & \text{if } \mathbf{y} \text{ is continuous} \end{cases}$$

where $\mathcal{Y}$ stands for the states of the target space of random variable Y.

- Marginalization property.

Sum Rule (2/2)

For $\mathbf{x} = [x_1, \ldots, x_D]^\top$, the marginal

$$p(x_i) = \int p(x_1, \ldots, x_D) \mathrm{d}\mathbf{x}_{-i}$$

, where "$-i$" means all except i.

Product Rule

Sum Rule

$$p(\mathbf{x}, \mathbf{y}) = p(\mathbf{y} \mid \mathbf{x}) p(\mathbf{x})$$

Outline

Bayes' Theorem

Bayes' Theorem

$$\underbrace{p(\mathbf{x} \mid \mathbf{y})}_{\text{posterior}} = \frac{\overbrace{p(\mathbf{y} \mid \mathbf{x})}^{\text{likelihood}} \overbrace{p(\mathbf{x})}^{\text{prior}}}{\underbrace{p(\mathbf{y})}_{\text{evidence}}}.$$

- Prior: subjective prior knowledge (before observing data).
- Likelihood $p(\mathbf{y} \mid \mathbf{x})$: the probability of $\mathbf{y}$ if we were to know the latent variable $\mathbf{x}$.
  - We call it "the likelihood of $\mathbf{x}$".
- Posterior $p(\mathbf{x} \mid \mathbf{y})$: the quantity that we know about $\mathbf{x}$ after having observed $\mathbf{y}$.

Marginal Likelihood/Evidence

$$p(\mathbf{y}) := \sum_{\mathbf{x} \in \mathcal{X}} p(\mathbf{y} \mid \mathbf{x}) p(\mathbf{x}) = \mathbb{E}_X[p(\mathbf{y} \mid \mathbf{x})]$$

$$p(\mathbf{y}) := \int_{\mathbf{x} \in \mathcal{X}} p(\mathbf{y} \mid \mathbf{x}) p(\mathbf{x}) \mathrm{d}\mathbf{x} = \mathbb{E}_X[p(\mathbf{y} \mid \mathbf{x})].$$

Outline

Expected Value

Expected value

The expected value of a function $g : \mathbb{R} \mapsto \mathbb{R}$ of a random variable $X \sim p(x)$ is

$$\mathbb{E}_X[g(x)] = \int_{\mathcal{X}} g(x)p(x)\mathrm{d}x,$$

or

$$\mathbb{E}_X[g(x)] = \sum_{x \in \mathcal{X}} g(x)p(x).$$

Expected Value

Expected value

The expected value of a function $g : \mathbb{R} \mapsto \mathbb{R}$ of a random variable $X \sim p(x)$ is

$$\mathbb{E}_X[g(x)] = \int_{\mathcal{X}} g(x)p(x)\mathrm{d}x,$$

or

$$\mathbb{E}_X[g(x)] = \sum_{x \in \mathcal{X}} g(x)p(x).$$

Multivariate X

$$\mathbb{E}_X[g(\mathbf{x})] = \begin{bmatrix} \mathbb{E}_{X_1}[g(x_1)] \\ \vdots \\ \mathbb{E}_{X_D}[g(x_D)] \end{bmatrix} \in \mathbb{R}^D,$$

where $\mathbb{E}_{X_d}$: taking the expectation w.r.t. the x_d.

Linearity of Expectation

Let $f(\mathbf{x}) = ag(\mathbf{x}) + bh(\mathbf{x})$ for $a, b \in \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^D$.

$$\begin{aligned}
\mathbb{E}_X[f(\mathbf{x})] &= \int f(\mathbf{x})p(\mathbf{x})\mathrm{d}x \\
&= \int [ag(\mathbf{x}) + bh(\mathbf{x})]]\mathrm{d}x \\
&= a\int g(\mathbf{x})p(\mathbf{x})\mathrm{d}x + b\int h(\mathbf{x})p(\mathbf{x})\mathrm{d}x \\
&= a\mathbb{E}_X[g(\mathbf{x})] + b\mathbb{E}_X[h(\mathbf{x})]
\end{aligned}$$

Covariance

The (univariate) coveriance between two univariate random variables $X, Y \in \mathbb{R}$ is

$$\text{Cov}_{X,Y}[x, y] := \mathbb{E}_{X,Y}[(x - \mathbb{E}_X[x])(y - \mathbb{E}_Y[y]).$$

Omit the subscript.

$$\text{Cov}[x, y] := \mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y].$$

Covariance

The (univariate) coveriance between two univariate random variables $X, Y \in \mathbb{R}$ is

$$\text{Cov}_{X,Y}[x, y] := \mathbb{E}_{X,Y}[(x - \mathbb{E}_X[x])(y - \mathbb{E}_Y[y]).$$

Omit the subscript.

$$\text{Cov}[x, y] := \mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y].$$

Note that

$$\text{Cov}[x, x] := \mathbb{E}[x^2] - (\mathbb{E}[x])^2$$

is the variance and denoted by $\mathbb{V}_X[x]$ and $\sqrt{\text{Cov}[x, x]}$ denoted by $\sigma(x)$ is called the standard deviation.

Covariance of Multivariate R.V.'s

Covariance (Multivariate)

Consider random variables X and Y with states $\mathbf{x} \in \mathbb{R}^D$ and $\mathbf{y} \in \mathbb{R}^E$. The covariance between X and Y:

$$\text{Cov}[\mathbf{x}, \mathbf{y}] =$$

Covariance of Multivariate R.V.'s

Covariance (Multivariate)

Consider random variables X and Y with states $\mathbf{x} \in \mathbb{R}^D$ and $\mathbf{y} \in \mathbb{R}^E$. The covariance between X and Y:

$$\text{Cov}[\mathbf{x}, \mathbf{y}] = \mathbb{E}[\mathbf{x}\mathbf{y}^\top] - \mathbb{E}[\mathbf{x}]\mathbb{E}[\mathbf{y}]^\top$$

Covariance of Multivariate R.V.'s

Covariance (Multivariate)

Consider random variables X and Y with states $\mathbf{x} \in \mathbb{R}^D$ and $\mathbf{y} \in \mathbb{R}^E$. The covariance between X and Y:

$$\text{Cov}[\mathbf{x}, \mathbf{y}] = \mathbb{E}[\mathbf{x}\mathbf{y}^\top] - \mathbb{E}[\mathbf{x}]\mathbb{E}[\mathbf{y}]^\top = \text{Cov}[\mathbf{y}, \mathbf{x}]^\top \in \mathbb{R}^{D \times E}.$$

Variance (Multivariate)

Variance (Multivariate)

The variance of a random variables X with states $\mathbf{x} \in \mathbb{R}^D$ and mean $\boldsymbol{\mu} \in \mathbb{R}^D$ is

$$\mathbb{V}_X[\mathbf{x}] = \mathrm{Cov}_X[\mathbf{x}, \mathbf{x}] = \mathbb{E}_X[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top]$$

Variance (Multivariate)

Variance (Multivariate)

The variance of a random variables X with states $\mathbf{x} \in \mathbb{R}^D$ and mean $\boldsymbol{\mu} \in \mathbb{R}^D$ is

$$\mathbb{V}_X[\mathbf{x}] = \mathrm{Cov}_X[\mathbf{x}, \mathbf{x}] = \mathbb{E}_X[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top] = \mathbb{E}_X[\mathbf{x}\mathbf{x}^\top] - \mathbb{E}_X[\mathbf{x}]\mathbb{E}_X[\mathbf{x}]^\top$$

Variance (Multivariate)

Variance (Multivariate)

The variance of a random variables X with states $\mathbf{x} \in \mathbb{R}^D$ and mean $\boldsymbol{\mu} \in \mathbb{R}^D$ is

$$\begin{aligned}\mathbb{V}_X[\mathbf{x}] &= \mathrm{Cov}_X[\mathbf{x},\mathbf{x}] = \mathbb{E}_X[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\top] = \mathbb{E}_X[\mathbf{x}\mathbf{x}^\top] - \mathbb{E}_X[\mathbf{x}]\mathbb{E}_X[\mathbf{x}]^\top \\ &= \begin{bmatrix} \mathrm{Cov}[x_1,x_1] & \mathrm{Cov}[x_1,x_2] & \cdots & \mathrm{Cov}[x_1,x_D] \\ \mathrm{Cov}[x_2,x_1] & \mathrm{Cov}[x_2,x_2] & \cdots & \mathrm{Cov}[x_2,x_D] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{Cov}[x_D,x_1] & \mathrm{Cov}[x_D,x_2] & \cdots & \mathrm{Cov}[x_D,x_D] \end{bmatrix}.\end{aligned}$$

Variance (Multivariate)

Variance (Multivariate)

The variance of a random variables X with states $\mathbf{x} \in \mathbb{R}^D$ and mean $\boldsymbol{\mu} \in \mathbb{R}^D$ is

$$\begin{aligned}\mathbb{V}_X[\mathbf{x}] &= \mathrm{Cov}_X[\mathbf{x},\mathbf{x}] = \mathbb{E}_X[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\top] = \mathbb{E}_X[\mathbf{x}\mathbf{x}^\top] - \mathbb{E}_X[\mathbf{x}]\mathbb{E}_X[\mathbf{x}]^\top \\ &= \begin{bmatrix} \mathrm{Cov}[x_1,x_1] & \mathrm{Cov}[x_1,x_2] & \cdots & \mathrm{Cov}[x_1,x_D] \\ \mathrm{Cov}[x_2,x_1] & \mathrm{Cov}[x_2,x_2] & \cdots & \mathrm{Cov}[x_2,x_D] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{Cov}[x_D,x_1] & \mathrm{Cov}[x_D,x_2] & \cdots & \mathrm{Cov}[x_D,x_D] \end{bmatrix}.\end{aligned}$$

- The covariance matrix of the multivariate X.

Correlation

Correlation

The correlation between two random variables X, Y is

$$\text{corr}[x, y] = \frac{\text{Cov}[x, y]}{\sqrt{\mathbb{V}[x]\mathbb{V}[y]}} \in [-1, 1].$$

Empirical Means & Covariances

In machine learning, we need to learn from empirical observations of data.

Empirical Mean & Covariance

The empirical mean vector: arithmetic average of the observations for each variable:

$$\bar{\mathbf{x}} := \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}_i,$$

for $\mathbf{x}_i \in \mathbb{R}^D$. The empirical covariance matrix is a $D \times D$ matrix

$$\boldsymbol{\Sigma} := \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^\top.$$

Empirical Means & Covariances

In machine learning, we need to learn from empirical observations of data.

Empirical Mean & Covariance

The empirical mean vector: arithmetic average of the observations for each variable:

$$\bar{\mathbf{x}} := \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}_i,$$

for $\mathbf{x}_i \in \mathbb{R}^D$. The empirical covariance matrix is a $D \times D$ matrix

$$\boldsymbol{\Sigma} := \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^\top.$$

- $\boldsymbol{\Sigma}$ is symmetric, positive semidefinite.

Computing the Empirical Variance

Approaches:

1. $\mathbb{V}_X[x] := \mathbb{E}_X[(x - \mu)^2]$.
2. $\mathbb{V}_X[x] = \mathbb{E}_X[x^2] - (\mathbb{E}_X[x])^2$.
   - One-pass; more efficient
3. Averaging pairwise differences between all pairs of observations.

$$\frac{1}{N^2} \sum_{i,j=1}^{N} (x_i - x_j)^2 = 2 \left[\frac{1}{N} \sum_{i=1}^{N} x_i^2 - \left(\frac{1}{N} \sum_{i=1}^{N} x_i \right)^2 \right].$$

Computing the Empirical Variance

Approaches:

1. $\mathbb{V}_X[x] := \mathbb{E}_X[(x-\mu)^2]$.
2. $\mathbb{V}_X[x] = \mathbb{E}_X[x^2] - (\mathbb{E}_X[x])^2$.
   - One-pass; more efficient
3. Averaging pairwise differences between all pairs of observations.

$$\frac{1}{N^2}\sum_{i,j=1}^{N}(x_i - x_j)^2 = 2\left[\frac{1}{N}\sum_{i=1}^{N}x_i^2 - \left(\frac{1}{N}\sum_{i=1}^{N}x_i\right)^2\right].$$

   - Twice of the 2nd approach.
   - Interesting perspective to compute the left-hand side target.

Outline

Basic Rules

Simple Rules & Exercise

Consider two random variables X, Y with states $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$. Then,

$$\begin{aligned} \mathbb{E}[\mathbf{x} \pm \mathbf{y}] &= \mathbb{E}[\mathbf{x}] \pm \mathbb{E}[\mathbf{y}] \\ \mathbb{V}[\mathbf{x} \pm \mathbf{y}] &= \mathbb{V}[\mathbf{x}] \pm \mathbb{V}[\mathbf{y}] \pm \mathrm{Cov}[\mathbf{x}, \mathbf{y}] \pm \mathrm{Cov}[\mathbf{y}, \mathbf{x}] \quad \text{(Exercise)}. \end{aligned}$$

- **Note:** For a constant vector $\mathbf{b} \in \mathbb{R}^D$, $\mathbb{V}(\mathbf{x} \pm \mathbf{b}) = \mathbb{V}[\mathbf{x}]$ because $\mathbb{V}[\mathbf{b}] = \mathbb{E}[\mathbf{b}\mathbf{b}^\top] - \mathbb{E}[\mathbf{b}]\mathbb{E}[\mathbf{b}]^\top = \mathbf{b}\mathbf{b}^\top - \mathbf{b}\mathbf{b}^\top = \mathbf{0}$ and

$$\mathrm{Cov}(\mathbf{x}, \mathbf{b})$$

Basic Rules

Simple Rules & Exercise

Consider two random variables X, Y with states $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$. Then,

$$\begin{aligned} \mathbb{E}[\mathbf{x} \pm \mathbf{y}] &= \mathbb{E}[\mathbf{x}] \pm \mathbb{E}[\mathbf{y}] \\ \mathbb{V}[\mathbf{x} \pm \mathbf{y}] &= \mathbb{V}[\mathbf{x}] \pm \mathbb{V}[\mathbf{y}] \pm \mathrm{Cov}[\mathbf{x}, \mathbf{y}] \pm \mathrm{Cov}[\mathbf{y}, \mathbf{x}] \quad \text{(Exercise)}. \end{aligned}$$

- **Note:** For a constant vector $\mathbf{b} \in \mathbb{R}^D$, $\mathbb{V}(\mathbf{x} \pm \mathbf{b}) = \mathbb{V}[\mathbf{x}]$ because $\mathbb{V}[\mathbf{b}] = \mathbb{E}[\mathbf{b}\mathbf{b}^\top] - \mathbb{E}[\mathbf{b}]\mathbb{E}[\mathbf{b}]^\top = \mathbf{b}\mathbf{b}^\top - \mathbf{b}\mathbf{b}^\top = \mathbf{0}$ and

$$\mathrm{Cov}(\mathbf{x}, \mathbf{b}) = \mathbb{E}[\mathbf{x}\mathbf{b}^\top] - \mathbb{E}[\mathbf{x}]\mathbb{E}[\mathbf{b}]^\top$$

Basic Rules

Simple Rules & Exercise

Consider two random variables X, Y with states $\mathbf{x}, \mathbf{y} \in \mathbb{R}^D$. Then,

$$\begin{aligned} \mathbb{E}[\mathbf{x} \pm \mathbf{y}] &= \mathbb{E}[\mathbf{x}] \pm \mathbb{E}[\mathbf{y}] \\ \mathbb{V}[\mathbf{x} \pm \mathbf{y}] &= \mathbb{V}[\mathbf{x}] \pm \mathbb{V}[\mathbf{y}] \pm \mathrm{Cov}[\mathbf{x}, \mathbf{y}] \pm \mathrm{Cov}[\mathbf{y}, \mathbf{x}] \quad \text{(Exercise)}. \end{aligned}$$

- **Note:** For a constant vector $\mathbf{b} \in \mathbb{R}^D$, $\mathbb{V}(\mathbf{x} \pm \mathbf{b}) = \mathbb{V}[\mathbf{x}]$ because $\mathbb{V}[\mathbf{b}] = \mathbb{E}[\mathbf{b}\mathbf{b}^\top] - \mathbb{E}[\mathbf{b}]\mathbb{E}[\mathbf{b}]^\top = \mathbf{b}\mathbf{b}^\top - \mathbf{b}\mathbf{b}^\top = \mathbf{0}$ and

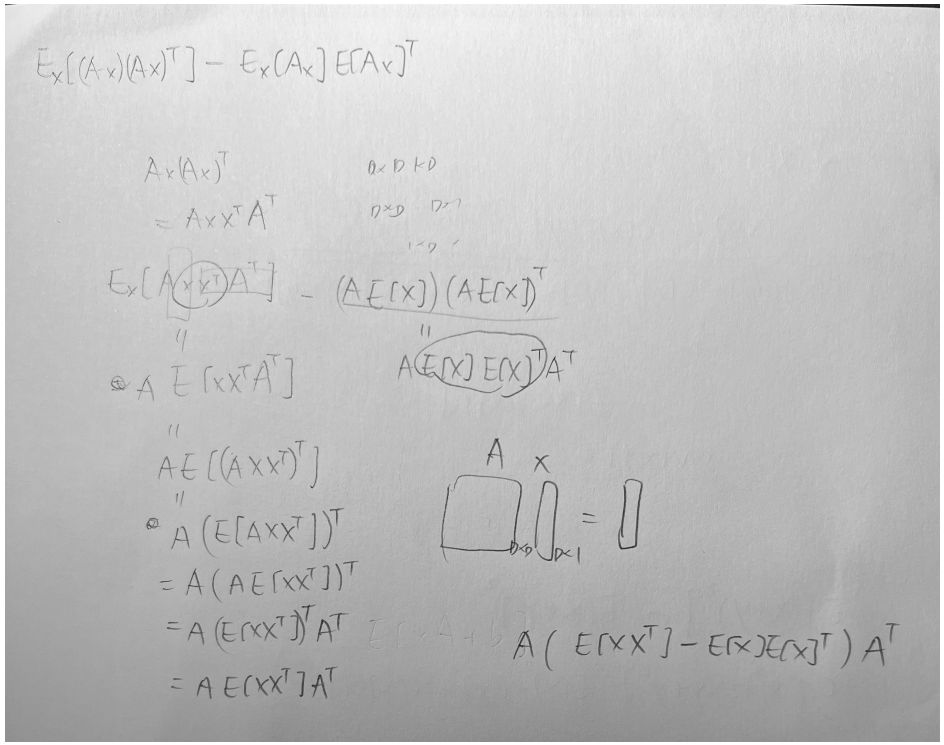
$$\mathrm{Cov}(\mathbf{x}, \mathbf{b}) = \mathbb{E}[\mathbf{x}\mathbf{b}^\top] - \mathbb{E}[\mathbf{x}]\mathbb{E}[\mathbf{b}]^\top = \mathbb{E}[\mathbf{x}]\mathbf{b}^\top - \mathbb{E}[\mathbf{x}]\mathbf{b}^\top = \mathbf{0}.$$

- **Question:** Why does the second equality hold?

Affine Transformation of r.v.'s (1/2)

Consider $\mathbf{y} = \boldsymbol{A}\mathbf{x} + \mathbf{b}$ and let $\boldsymbol{\Sigma} := \mathbb{V}_X[\mathbf{x}]$.

$$\begin{aligned} \mathbb{E}_Y[\mathbf{y}] &= \mathbb{E}_X[\boldsymbol{A}\mathbf{x} + \mathbf{b}] = \boldsymbol{A}\mathbb{E}_X[\mathbf{x}] + \mathbf{b} \\ \mathbb{V}_Y[\mathbf{y}] &= \mathbb{V}_X[\boldsymbol{A}\mathbf{x} + \mathbf{b}] = \mathbb{V}_X[\boldsymbol{A}\mathbf{x}] = \boldsymbol{A}\mathbb{V}_X[\mathbf{x}]\boldsymbol{A}^\top = \boldsymbol{A}\boldsymbol{\Sigma}\boldsymbol{A}^\top. \end{aligned}$$



Affine Transformation of r.v.'s (2/2)

Furthermore, let $\boldsymbol{\mu} := \mathbb{E}_X[\mathbf{x}]$ and $\boldsymbol{\Sigma} := \mathbb{V}_X[\mathbf{x}]$.

$$\begin{aligned}
\text{Cov}[\mathbf{x}, \mathbf{y}] &= \mathbb{E}[\mathbf{x}(\boldsymbol{A}\mathbf{x} + \mathbf{b})^\top] - \mathbb{E}[\mathbf{x}]\mathbb{E}[\boldsymbol{A}\mathbf{x} + \mathbf{b}]^\top \\
&= \boldsymbol{\mu}\mathbf{b}^\top + \mathbb{E}[\mathbf{x}\mathbf{x}^\top]\boldsymbol{A}^\top - \boldsymbol{\mu}\mathbf{b}^\top - \boldsymbol{\mu}\boldsymbol{\mu}^\top\boldsymbol{A}^\top \\
&= (\mathbb{E}[\mathbf{x}\mathbf{x}^\top] - \boldsymbol{\mu}\boldsymbol{\mu}^\top)\boldsymbol{A}^\top \\
&= \boldsymbol{\Sigma}\boldsymbol{A}^\top.
\end{aligned}$$

Outline

(Statistically) Independent

Two random variables X, Y are statistically independent if and only if

$$p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x})p(\mathbf{y}).$$

If X, Y are independent, then

- $p(\mathbf{y} \mid \mathbf{x}) = p(\mathbf{y})$.
- $p(\mathbf{x} \mid \mathbf{y}) = p(\mathbf{x})$.
- $\mathbb{V}_{X,Y}[\mathbf{x} + \mathbf{y}] = \mathbb{V}_X[\mathbf{x}] + \mathbb{V}_Y[\mathbf{y}]$.
- $\mathrm{Cov}_{X,Y}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$.

Note that $\mathrm{Cov}_{X,Y}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$ does NOT necessarily imply that X and Y are independent.

See Example (6.5).

Conditional Independence

Two random variables X, Y are conditionally independent given Z if and only if

$$p(\mathbf{x}, \mathbf{y} \mid \mathbf{z}) = p(\mathbf{x} \mid \mathbf{z}) p(\mathbf{y} \mid \mathbf{z}).$$

for all $\mathbf{z} \in \mathcal{Z}$.

By the product rule, we can have

$$p(\mathbf{x}, \mathbf{y} \mid \mathbf{z}) = p(\mathbf{x} \mid \mathbf{y}, \mathbf{z}) p(\mathbf{y} \mid \mathbf{z}).$$

Thus,

$$p(\mathbf{x} \mid \mathbf{y}, \mathbf{z}) = p(\mathbf{x} \mid \mathbf{z}).$$

Heads Up

If X, Y are independent, then $\mathbb{V}_{X,Y}[\mathbf{x}+\mathbf{y}] = \mathbb{V}_X[\mathbf{x}] + \mathbb{V}_Y[\mathbf{y}]$.

$\because \quad \text{Cov}_{X,Y}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$

Discussions