Mathematics for Machine Learning

— Probability & Distributions (Supplementary):

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

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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

- Sum & Product Rule
- Bayes' Theorem
- Means & Covariances
- Sums & Transformations of Random Variables
- 5 Statistical Independence

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- 2 Bayes' Theorem
- Means & Covariances
- 4 Sums & Transformations of Random Variables
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Sum Rule (1/2)

- x, y: random variables (vectors).
- p(x, y): joint distribution of x, y.
- $p(y \mid x)$: conditional probability of **y** given **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 ${\cal Y}$ stands for the states of the target space of random variable ${\it Y}$.

• Marginalization property.

Sum Rule (2/2)

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

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

, where "-i" means all except i.

Product Rule

Product Rule

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

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Bayes' Theorem

Bayes' Theorem

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

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

Marginal Likelihood/Evidence

$$\begin{split} \rho(\mathbf{y}) &:= \sum_{\mathbf{x} \in \mathcal{X}} \rho(\mathbf{y} \mid \mathbf{x}) \rho(\mathbf{x}) = \mathbb{E}_{X} [\rho(\mathbf{y} \mid \mathbf{x})] \\ \rho(\mathbf{y}) &:= \int_{\mathbf{x} \in \mathcal{X}} \rho(\mathbf{y} \mid \mathbf{x}) \rho(\mathbf{x}) \mathrm{d}\mathbf{x} = \mathbb{E}_{X} [\rho(\mathbf{y} \mid \mathbf{x})]. \end{split}$$

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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

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

or

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

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Multivariate $X = [X_1, \dots, X_D]^{\top}$

$$\mathbb{E}_{X}[g(\mathbf{x})] = \left[egin{array}{c} \mathbb{E}_{X_{1}}[g(x_{1})] \ dots \ \mathbb{E}_{X_{D}}[g(x_{D})] \end{array}
ight] \in \mathbb{R}^{D},$$

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

Expected Value (contd.)

Mean

For $\mathbf{x} \in \mathbb{R}^D$,

$$\mathbb{E}_{X}[\mathbf{x}] = \left[egin{array}{c} \mathbb{E}_{X_1}[x_1] \ dots \ \mathbb{E}_{X_D}[x_D] \end{array}
ight] \in \mathbb{R}^D,$$

where

- $\mathbb{E}_{X_d}[x_d] = \int_{\mathcal{X}} x_d p(x_d) dx_d$ if X is continuous;
- $\mathbb{E}_{X_d}[x_d] = \sum_{x_i \in \mathcal{X}} x_i p(x_d = x_i) dx_d$ if X is discrete.

Linearity of Expectation

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

$$\mathbb{E}_X[f(\mathbf{x})] = \int f(\mathbf{x})p(\mathbf{x})d\mathbf{x}$$

$$= \int [ag(\mathbf{x}) + bh(\mathbf{x})]d\mathbf{x}$$

$$= a \int g(\mathbf{x})p(\mathbf{x})d\mathbf{x} + b \int h(\mathbf{x})p(\mathbf{x})d\mathbf{x}$$

$$= a\mathbb{E}_X[g(\mathbf{x})] + b\mathbb{E}_X[h(\mathbf{x})].$$

Linearity of Expectation (Discrete Case)

Let
$$f(\mathbf{x}) = ag(\mathbf{x}) + bh(\mathbf{x})$$
 for $a, b \in \mathbb{R}$ and $\mathbf{x} \in \mathcal{X}$.
$$\mathbb{E}_X[f(\mathbf{x})] = \sum_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})p(\mathbf{x})$$

$$= \sum_{\mathbf{x} \in \mathcal{X}} [ag(\mathbf{x}) + bh(\mathbf{x})]p(\mathbf{x})$$

$$= a\sum_{\mathbf{x} \in \mathcal{X}} g(\mathbf{x})p(\mathbf{x}) + b\sum_{\mathbf{x} \in \mathcal{X}} h(\mathbf{x})p(\mathbf{x})$$

$$= a\mathbb{E}_X[g(\mathbf{x})] + b\mathbb{E}_X[h(\mathbf{x})].$$

Covariance

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

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

Omit the subscript.

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

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Omit the subscript.

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

Note that

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

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:

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

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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:

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

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

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

Variance (Multivariate)

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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

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

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

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

$$= \begin{bmatrix} \operatorname{Cov}[x_{1}, x_{1}] & \operatorname{Cov}[x_{1}, x_{2}] & \cdots & \operatorname{Cov}[x_{1}, x_{D}] \\ \operatorname{Cov}[x_{2}, x_{1}] & \operatorname{Cov}[x_{2}, x_{2}] & \cdots & \operatorname{Cov}[x_{2}, x_{D}] \\ \vdots & \vdots & \ddots & \vdots \\ \operatorname{Cov}[x_{D}, x_{1}] & \operatorname{Cov}[x_{D}, x_{2}] & \cdots & \operatorname{Cov}[x_{D}, x_{D}] \end{bmatrix}.$$

• The covariance matrix of the multivariate X.

Correlation

Correlation

The correlation between two random variables X, Y is

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

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

$$oldsymbol{\Sigma} := rac{1}{N} \sum_{i=1}^N (\mathbf{x}_i - ar{\mathbf{x}}) (\mathbf{x}_i - ar{\mathbf{x}})^{ op}.$$

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 \bullet Σ 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
- Averaging pairwise differences between all pairs of observations.

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

Computing the Empirical Variance

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 - One-pass; more efficient
- 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.

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Basic Rules

Simple Rules & Exercise

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

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

• 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 $\mathsf{Cov}(\mathbf{x}, \mathbf{b})$

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

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

Basic Rules

Simple Rules & Exercise

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

$$\begin{split} \mathbb{E}[\mathbf{x} \pm \mathbf{y}] &= \mathbb{E}[\mathbf{x}] \pm \mathbb{E}[\mathbf{y}] \\ \mathbb{V}[\mathbf{x} \pm \mathbf{y}] &= \mathbb{V}[\mathbf{x}] + \mathbb{V}[\mathbf{y}] \pm \mathsf{Cov}[\mathbf{x}, \mathbf{y}] \pm \mathsf{Cov}[\mathbf{y}, \mathbf{x}] \end{aligned}$$
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• 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

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

• Question: Why does the second equality hold?

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

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

$$\mathbb{E}_{Y}[y] = \mathbb{E}_{X}[Ax + b] = A\mathbb{E}_{X}[x] + b$$

$$\mathbb{V}_{Y}[y] = \mathbb{V}_{X}[Ax + b] = \mathbb{V}_{X}[Ax] = A\mathbb{V}_{X}[x]A^{\top} = A\Sigma A^{\top}.$$

$$\mathbb{V}_X[\mathbf{A}\mathbf{x}] = \mathbb{E}_X[(\mathbf{A}\mathbf{x})(\mathbf{A}\mathbf{x})^{\top}]$$

$$\mathbb{V}_X[\mathbf{A}\mathbf{x}] = \mathbb{E}_X[(\mathbf{A}\mathbf{x})(\mathbf{A}\mathbf{x})^{\top}] = \mathbb{E}_X[\mathbf{A}\mathbf{x}\mathbf{x}^{\top}\mathbf{A}^{\top}]$$

$$\mathbb{V}_X[\mathbf{A}\mathbf{x}] = \mathbb{E}_X[(\mathbf{A}\mathbf{x})(\mathbf{A}\mathbf{x})^\top] = \mathbb{E}_X[\mathbf{A}\mathbf{x}\mathbf{x}^\top\mathbf{A}^\top] = \mathbf{A}\mathbb{E}_X[\mathbf{x}\mathbf{x}^\top\mathbf{A}^\top]$$

$$\begin{aligned} \mathbb{V}_X[\mathbf{A}\mathbf{x}] &= \mathbb{E}_X[(\mathbf{A}\mathbf{x})(\mathbf{A}\mathbf{x})^\top] = \mathbb{E}_X[\mathbf{A}\mathbf{x}\mathbf{x}^\top\mathbf{A}^\top] = \mathbf{A}\mathbb{E}_X[\mathbf{x}\mathbf{x}^\top\mathbf{A}^\top] \\ &= \mathbf{A}(\mathbb{E}_X[\mathbf{A}\mathbf{x}\mathbf{x}^\top])^\top \end{aligned}$$

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= \mathbf{A}(\mathbb{E}_{X}[\mathbf{A}\mathbf{x}\mathbf{x}^{\top}])^{\top} = \mathbf{A}(\mathbf{A}\mathbb{E}_{X}[\mathbf{x}\mathbf{x}^{\top}])^{\top} = \mathbf{A}\mathbb{E}_{X}[\mathbf{x}\mathbf{x}^{\top}]\mathbf{A}^{\top}
= \mathbf{A}\mathbb{V}_{X}[\mathbf{x}]\mathbf{A}^{\top}.$$

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

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

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

$$= \mu \mathbf{b}^{\top} + \mathbb{E}[\mathbf{x}\mathbf{x}^{\top}]\mathbf{A}^{\top} - \mu \mathbf{b}^{\top} - \mu \mu^{\top}\mathbf{A}^{\top}$$

$$= (\mathbb{E}[\mathbf{x}\mathbf{x}^{\top}] - \mu \mu^{\top})\mathbf{A}^{\top}$$

$$= \Sigma \mathbf{A}^{\top}.$$

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(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

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

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

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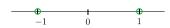
• Consider a random variable X with $\mathbb{E}_X[x] = 0$ and also $\mathbb{E}_X[x^3] = 0$.

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

- Consider a random variable X with $\mathbb{E}_X[x] = 0$ and also $\mathbb{E}_X[x^3] = 0$.
- Let $y = x^2$. Hence, Y is dependent on X.

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

- Consider a random variable X with $\mathbb{E}_X[x] = 0$ and also $\mathbb{E}_X[x^3] = 0$.
- Let $y = x^2$. Hence, Y is dependent on X.
- $Cov[x, y] = \mathbb{E}[xy] \mathbb{E}[x]\mathbb{E}[y] = \mathbb{E}[x^3] = 0.$



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

$$:: Cov_{X,Y}(\mathbf{x},\mathbf{y}) = \mathbf{0}$$

Discussions