

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

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

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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

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

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

- **Marginalization property.**

Sum Rule (2/2)

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

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

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

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

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

Marginal Likelihood/Evidence

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

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Expected Value

Expected value

The expected value of a function $g : \mathbb{R} \rightarrow \mathbb{R}$ 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 $X = [X_1, \dots, X_D]^\top$

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

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

Expected Value (contd.)

Mean

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

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

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 $\mathbf{x} \in \mathbb{R}^D$.

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

Linearity of Expectation (Discrete Case)

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

$$\begin{aligned}\mathbb{E}_{\mathcal{X}}[f(\mathbf{x})] &= \sum_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})p(\mathbf{x}) \\ &= \sum_{\mathbf{x} \in \mathcal{X}} [ag(\mathbf{x}) + bh(\mathbf{x})]p(\mathbf{x}) \\ &= a \sum_{\mathbf{x} \in \mathcal{X}} g(\mathbf{x})p(\mathbf{x}) + b \sum_{\mathbf{x} \in \mathcal{X}} h(\mathbf{x})p(\mathbf{x}) \\ &= a\mathbb{E}_{\mathcal{X}}[g(\mathbf{x})] + b\mathbb{E}_{\mathcal{X}}[h(\mathbf{x})].\end{aligned}$$

Covariance

The (univariate) covariance 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.

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

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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 :

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

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

Variance (Multivariate)

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

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

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- 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

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

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

- Σ is symmetric, positive semidefinite.

Computing the Empirical Variance (1D Example)

Approaches:

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

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

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- Twice of the 2nd approach (left-hand side: $O(N^2)$).
- Interesting perspective to compute the left-hand side target.

Welford's Online Algorithm [1962]

- **Input:** Stream of observations x_1, x_2, \dots
 - **Output:** (population) variances σ^2 , and unbiased variance s^2 .
 - ① **Initialization:** $n \leftarrow 0, \mu \leftarrow 0, M_2 \leftarrow 0$;
 - ② for each x_i in stream, $i = 1, 2, \dots$
 - ① $n \leftarrow n + 1$;
 - ② $\delta \leftarrow x - \mu, \mu \leftarrow \mu + \delta/n$; /* empirical mean update */
 - ③ $\delta_2 \leftarrow x - \mu, M_2 \leftarrow M_2 + \delta \cdot \delta_2$ /* $M_2 = \sum_{i=1}^n (x_i - \mu_n)^2$ */
 - ③ **population variance:** $\sigma^2 \leftarrow M_2/n$ (valid for $n \geq 1$);
 - ④ **unbiased variance:** $s^2 \leftarrow M_2/(n-1)$ (valid for $n \geq 2$)
- Each increment δ and δ_2 are on the scale of the deviation or variance, not on the scale of x and x^2 .

Accuracy of Welford's Online Algorithm (Mean)

Setup. For a stream x_1, x_2, \dots , maintain $\mu_n :=$ mean after n , $M_2^{(n)} = \sum_{i=1}^n (x_i - \mu_n)^2$. Given $(\mu_{n-1}, M_2^{(n-1)})$ and new x_n ,

$$\delta = x_n - \mu_{n-1}, \quad \mu_n = \mu_{n-1} + \frac{\delta}{n}, \quad \delta_2 = x_n - \mu_n, \quad M_2^{(n)} = M_2^{(n-1)} + \delta \delta_2.$$

Claim (Mean exactness). $\mu_n = \frac{1}{n} \sum_{i=1}^n x_i$.

Proof

Base $n = 1$: $\mu_1 = x_1$. For the step,

$$\mu_n = \mu_{n-1} + \frac{x_n - \mu_{n-1}}{n} = \frac{(n-1)\mu_{n-1} + x_n}{n} = \frac{\sum_{i=1}^{n-1} x_i + x_n}{n} = \frac{1}{n} \sum_{i=1}^n x_i.$$

Accuracy of Welford's Online Algorithm (2nd Moment)

Claim. $M_2^{(n)} = \sum_{i=1}^n (x_i - \mu_n)^2$ is preserved by $M_2^{(n)} = M_2^{(n-1)} + \delta \delta_2$ with $\delta = x_n - \mu_{n-1}$ and $\delta_2 = x_n - \mu_n$.

Proof

Assume $M_2^{(n-1)} = \sum_{i=1}^{n-1} (x_i - \mu_{n-1})^2$. Then

$$\begin{aligned} \sum_{i=1}^n (x_i - \mu_n)^2 &= \sum_{i=1}^{n-1} [(x_i - \mu_{n-1}) + (\mu_{n-1} - \mu_n)]^2 + (x_n - \mu_n)^2 \\ &= \underbrace{\sum_{i=1}^{n-1} (x_i - \mu_{n-1})^2}_{M_2^{(n-1)}} + (n-1)(\mu_{n-1} - \mu_n)^2 + (x_n - \mu_n)^2, \end{aligned}$$

Accuracy of Welford's Online Algorithm (2nd Moment) Contd.

Since $\sum_{i=1}^{n-1} (x_i - \mu_{n-1}) = 0$. With $\mu_n - \mu_{n-1} = \delta/n$ and $\delta_2 = x_n - \mu_n = \delta(1 - 1/n)$,

$$\begin{aligned}(n-1)(\mu_{n-1} - \mu_n)^2 + (x_n - \mu_n)^2 &= \frac{(n-1)\delta^2}{n^2} + \frac{(n-1)^2\delta^2}{n^2} \\ &= \frac{(n-1)\delta^2}{n} \\ &= \delta\delta_2.\end{aligned}$$

Therefore $\sum_{i=1}^n (x_i - \mu_n)^2 = M_2^{(n-1)} + \delta\delta_2 = M_2^{(n)}$.

Consequences. Population variance: $\sigma^2 = M_2^{(n)}/n$ (for $n \geq 1$);
unbiased sample variance: $s^2 = M_2^{(n)}/(n-1)$ (for $n \geq 2$).

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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,

$$\mathbb{E}[\mathbf{x} \pm \mathbf{y}] = \mathbb{E}[\mathbf{x}] \pm \mathbb{E}[\mathbf{y}]$$

$$\mathbb{V}[\mathbf{x} \pm \mathbf{y}] = \mathbb{V}[\mathbf{x}] + \mathbb{V}[\mathbf{y}] \pm \text{Cov}[\mathbf{x}, \mathbf{y}] \pm \text{Cov}[\mathbf{y}, \mathbf{x}] \quad (\text{Exercise}).$$

- **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

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

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

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

$$\mathbb{E}[\mathbf{x} \pm \mathbf{y}] = \mathbb{E}[\mathbf{x}] \pm \mathbb{E}[\mathbf{y}]$$

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

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

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

$$\mathbb{E}_Y[\mathbf{y}] = \mathbb{E}_X[\mathbf{A}\mathbf{x} + \mathbf{b}] = \mathbf{A}\mathbb{E}_X[\mathbf{x}] + \mathbf{b}$$

$$\mathbb{V}_Y[\mathbf{y}] = \mathbb{V}_X[\mathbf{A}\mathbf{x} + \mathbf{b}] = \mathbb{V}_X[\mathbf{A}\mathbf{x}] = \mathbf{A}\mathbb{V}_X[\mathbf{x}]\mathbf{A}^\top = \mathbf{A}\mathbf{\Sigma}\mathbf{A}^\top.$$

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

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

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

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

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

Outline

- 1 Sum & Product Rule
- 2 Bayes' Theorem
- 3 Means & Covariances
- 4 Sums & Transformations of Random Variables
- 5 Statistical Independence**

(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

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

Remark

Note that $\text{Cov}_{X,Y}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$ 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 $\mathbb{E}_X[x^3] = 0$.

Remark

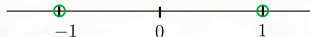
Note that $\text{Cov}_{X,Y}(\mathbf{x}, \mathbf{y}) = \mathbf{0}$ does NOT necessarily imply that X and Y are independent.

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- Let $y = x^2$. Hence, Y is **dependent on X** .

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- 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** .
- $\text{Cov}[x, y] = \mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y] = \mathbb{E}[x^3] = 0$.



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

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

Discussions