Mathematics for Machine Learning

— Probability & Distributions

Gaussian Distribution & Change of Variables/Inverse Transform

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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.*
  - *Arnold J. Insel, Lawrence E. Spence, Stephen H. Friedberg: Linear Algebra, 4th Edition. Prentice Hall. 2013.*
  - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra, 12th Edition. Wiley. 2019.*
- We could partially refer to the monograph:
  Francesco Orabona: A Modern Introduction to Online Learning. https://arxiv.org/abs/1912.13213

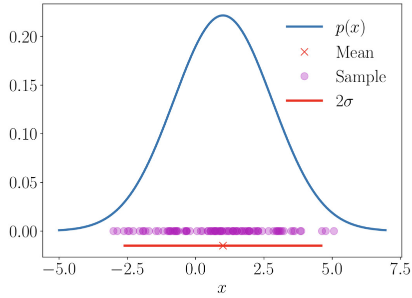
Outline

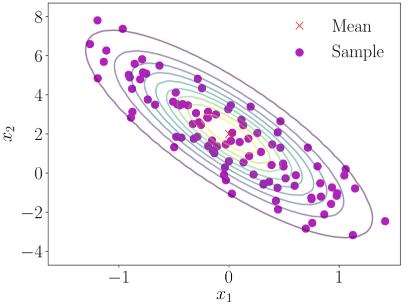
Outline

Introduction

- The Gaussian distribution (a.k.s. normal distribution) is the most well-studied probability distribution for continuous-valued random variables.
- Widely used in statistics and machine learning.

Gaussian Distributions Overlaid with Samples





Univariate & Multivariate Gaussian

The probability density functions.

Univariate

$$p(x \mid \mu, \sigma^2) = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right).$$

$\boldsymbol{\Sigma} = \mathbb{V}_X[\mathbf{x}] = \mathrm{Cov}_X[\mathbf{x}, \mathbf{x}]$.

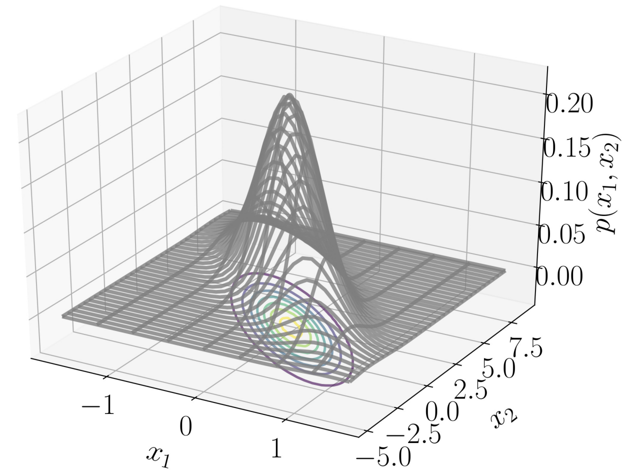
Multivariate

$$p(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}} \det(\boldsymbol{\Sigma})^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right),$$

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

We write $p(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$ or $X \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

Gaussian distribution of two random variables x_1, x_2.



Outline

Marginals and Conditionals of Gaussians

- Let X, Y be two multivariate random variables.
- Concatenate their states to be $[\mathbf{x}^\top, \mathbf{y}^\top]$.

$$p(\mathbf{x}, \mathbf{y}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{bmatrix}\right),$$

where $\boldsymbol{\Sigma}_{xx} = \mathrm{Cov}[\mathbf{x}, \mathbf{x}]$, $\boldsymbol{\Sigma}_{yy} = \mathrm{Cov}[\mathbf{y}, \mathbf{y}]$, $\boldsymbol{\Sigma}_{xy} = \mathrm{Cov}[\mathbf{x}, \mathbf{y}]$.

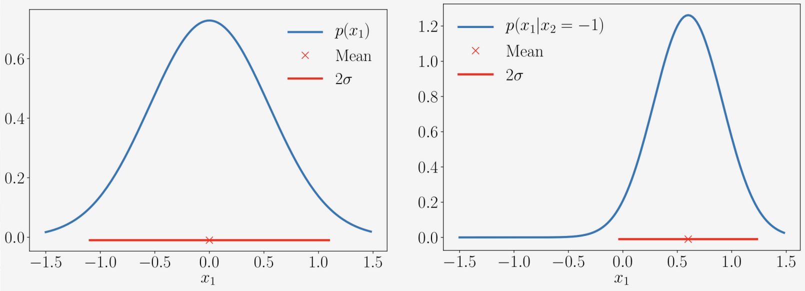
- By [Bishop 2006], the conditional distribution $p(\mathbf{x} \mid \mathbf{y})$ is also Gaussian.

$$\begin{aligned} p(\mathbf{x} \mid \mathbf{y}) &= \mathcal{N}(\boldsymbol{\mu}_{x|y}, \boldsymbol{\Sigma}_{x|y}) \\ \boldsymbol{\mu}_{x|y} &= \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}(\mathbf{y} - \boldsymbol{\mu}_y) \\ \boldsymbol{\Sigma}_{x|y} &= \boldsymbol{\Sigma}_{xx} - \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}\boldsymbol{\Sigma}_{yx}. \end{aligned}$$

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{y})\mathrm{d}\mathbf{y} = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}_x, \boldsymbol{\Sigma}_{xx}).$$

Example

Consider $$p(x_1, x_2) = \mathcal{N}\left(\begin{bmatrix} 0 \\ 2 \end{bmatrix}, \begin{bmatrix} 0.3 & -1 \\ -1 & 5 \end{bmatrix}\right).$$



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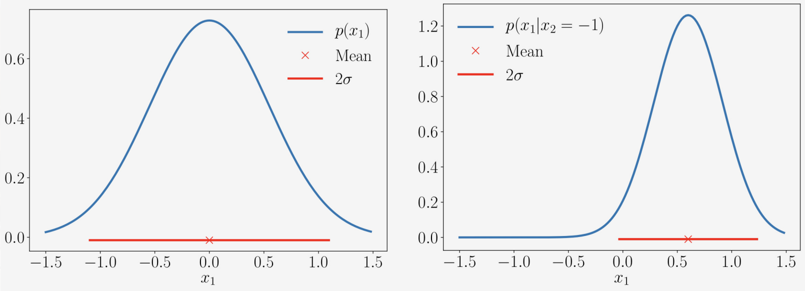

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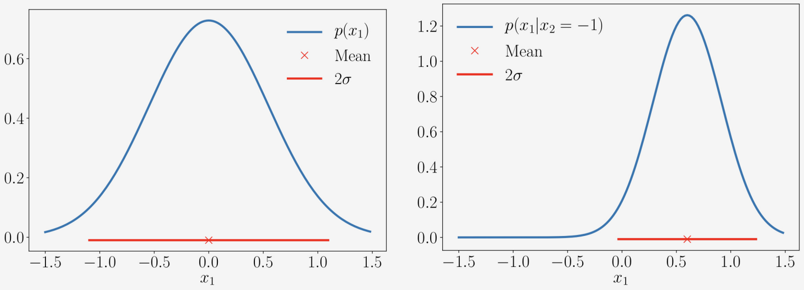

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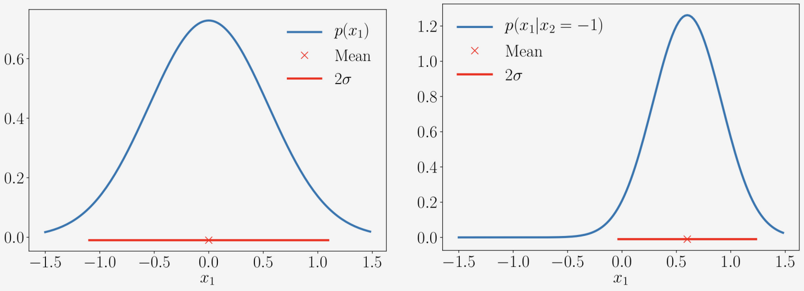

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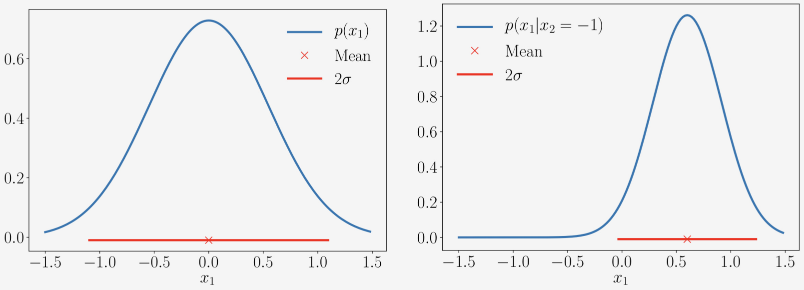

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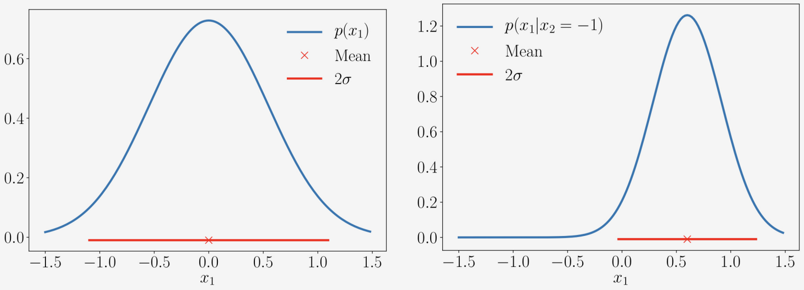

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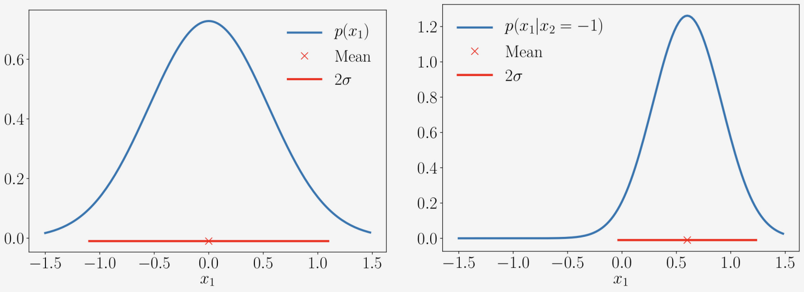

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Thus, $p(x_1 \mid x_2 = -1) = \mathcal{N}(0.6, 0.1)$, $\quad p(x_1) = \mathcal{N}(0, 0.3)$.

Outline

Sum of Gaussians

Say X, Y are two independent Gaussian random variables with

$$X \sim \mathcal{N}(\boldsymbol{\mu}_x, \boldsymbol{\Sigma}_x) \text{ and } Y \sim \mathcal{N}(\boldsymbol{\mu}_y, \boldsymbol{\Sigma}_y).$$

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

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Then $X + Y$ is also a Gaussian distribution with

$$X + Y \sim \mathcal{N}(\boldsymbol{\mu}_x + \boldsymbol{\mu}_y, \boldsymbol{\Sigma}_x + \boldsymbol{\Sigma}_y)$$

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Please recall $\mathbb{E}[\mathbf{x} + \mathbf{y}]$ and $\mathbb{V}[\mathbf{x} + \mathbf{y}]$.

Example

Linear Combination of Two Independent Gaussians

$$p(a\mathbf{x} + b\mathbf{y}) =$$

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$$p(a\mathbf{x} + b\mathbf{y}) = \mathcal{N}(a\boldsymbol{\mu}_{\mathbf{x}} + b\boldsymbol{\mu}_{\mathbf{y}},\ a^2\boldsymbol{\Sigma}_{\mathbf{x}} + b^2\boldsymbol{\Sigma}_{\mathbf{y}}).$$

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Theorem [Mixture of Two Univariate Gaussian Densities]

Consider a mixture of two univariate Gaussian densities

$$p(x) = \alpha p_1(x) + (1-\alpha)p_2(x)$$

for the mixture weight $0 < \alpha < 1$ and $(\mu_1, \sigma_1^2) \neq (\mu_2, \sigma_2^2)$. Then,

$$\begin{aligned} \mathbb{E}[x] &= \alpha\mu_1 + (1-\alpha)\mu_2 \\ \mathbb{V}[x] &= \left[\alpha\sigma_1^2 + (1-\alpha)\sigma_2^2\right] \\ &\quad + \left(\left[\alpha\mu_1^2 + (1-\alpha)\mu_2^2\right] - \left[\alpha\mu_1 + (1-\alpha)\mu_2\right]^2\right). \end{aligned}$$

Proof of the Theorem

Sketch:

1. $\mathbb{E}[x] = \int_{-\infty}^{\infty} xp(x)\mathrm{d}x = \int_{-\infty}^{\infty} (\alpha x p_1(x) + (1-\alpha)xp_2(x))\mathrm{d}x$
$= \alpha\mu_1 + (1-\alpha)\mu_2.$

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   - **Recall:** $\mathbb{V}_X[x] = \mathbb{E}_X[x^2] - (\mathbb{E}_X[x])^2$.

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Using ① & ② we can prove the theorem.

Linear Transformation by a Matrix (1/2)

$X \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$ and $\mathbf{y} = \boldsymbol{A}\mathbf{x}$

- The expectation: $\mathbb{E}[\mathbf{y}] = \mathbb{E}[\boldsymbol{A}\mathbf{x}] =$

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$$Y \sim \mathcal{N}(\boldsymbol{A}\boldsymbol{\mu}, \boldsymbol{A}\boldsymbol{\Sigma}\boldsymbol{A}^\top).$$

Linear Transformation by a Matrix (2/2)

Let's consider the reverse transformation.

$Y \sim \mathcal{N}(\boldsymbol{\mu}_y, \boldsymbol{\Sigma})$, $\mathbf{y} = \boldsymbol{A}\mathbf{x}$ for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^M$, a full rank $\boldsymbol{A} \in \mathbb{R}^{M \times N}$, $M \geq N$

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$$X \sim \mathcal{N}((\boldsymbol{A}^\top \boldsymbol{A})^{-1} \boldsymbol{A}^\top \mu_y, (\boldsymbol{A}^\top \boldsymbol{A})^{-1} \boldsymbol{A}^\top \Sigma \boldsymbol{A} (\boldsymbol{A}^\top \boldsymbol{A})^{-1}).$$

Exercise

Another example of *reverse transformation*.

$Y \sim \mathcal{N}(\boldsymbol{\mu}_y, \boldsymbol{\Sigma})$ and $\mathbf{y} = \boldsymbol{A}\mathbf{x}$ for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^M$, and $\boldsymbol{A}$ is invertible

- $p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid \boldsymbol{A}\mathbf{x}, \boldsymbol{\Sigma})$.
- Compute $\mathbb{E}[\mathbf{x}]$.
- Compute $\mathbb{V}[\mathbf{x}]$.
- Derive $X \sim \mathcal{N}(?,\ ?)$.

A Sampling Approach

We want to obtain samples from a multivariate $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

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- Then, define $\mathbf{y} = \boldsymbol{A}\mathbf{x} + \boldsymbol{\mu}$, where $\boldsymbol{A}\boldsymbol{I}\boldsymbol{A}^\top = \boldsymbol{A}\boldsymbol{A}^\top = \boldsymbol{\Sigma}$.
- To derive $\boldsymbol{A}$: Use Cholesky decomposition of the covariance matrix $\boldsymbol{\Sigma}$.
  - $\boldsymbol{A}$ will be triangular and efficient for computation.

Outline

Product of Gaussian Densities: Statement

Product of Gaussians

- Let $\mathbf{x} \in \mathbb{R}^D$, and consider two Gaussians

$$\mathcal{N}(\mathbf{x} \mid \mathbf{a}, \boldsymbol{A}), \qquad \mathcal{N}(\mathbf{x} \mid \mathbf{b}, \boldsymbol{B}),$$

where $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{D \times D}$ are positive definite.

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  where $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{D \times D}$ are positive definite.

- Their product can be written as

$$\mathcal{N}(\mathbf{x} \mid \mathbf{a}, \boldsymbol{A})\,\mathcal{N}(\mathbf{x} \mid \mathbf{b}, \boldsymbol{B}) = \rho\,\mathcal{N}(\mathbf{x} \mid \mathbf{m}, \boldsymbol{S}),$$

  with

$$\boldsymbol{S} = (\boldsymbol{A}^{-1} + \boldsymbol{B}^{-1})^{-1}, \qquad \mathbf{m} = \boldsymbol{S}(\boldsymbol{A}^{-1}\mathbf{a} + \boldsymbol{B}^{-1}\mathbf{b}),$$

  and

$$rho = \mathcal{N}(a \mid b, A + B) = \mathcal{N}(b \mid a, A + B).$$

Proof Step 1: Completing the Square

- Write both Gaussians explicitly:

$$\mathcal{N}(\mathbf{x} \mid \mathbf{a}, \boldsymbol{A}) = (2\pi)^{-D/2} \det(\boldsymbol{A})^{-1/2} \exp\Big(- \tfrac{1}{2}(\mathbf{x} - \mathbf{a})^\top \boldsymbol{A}^{-1}(\mathbf{x} - \mathbf{a})\Big),$$

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- Their product is

$$\mathcal{N}(\mathbf{x} \mid \mathbf{a}, \boldsymbol{A})\mathcal{N}(\mathbf{x} \mid \mathbf{b}, \boldsymbol{B}) = (2\pi)^{-D} \det(\boldsymbol{A})^{-1/2} \det(\boldsymbol{B})^{-1/2} \cdot \exp\Big(-\tfrac{1}{2}\big[(\mathbf{x}-\mathbf{a})^\top \boldsymbol{A}^{-1}(\mathbf{x}-\mathbf{a}) + (\mathbf{x}-\mathbf{b})^\top \boldsymbol{B}^{-1}(\mathbf{x}-\mathbf{b})\big]\Big).$$

Step 1: Completing the Square (cont.)

- Expand the exponent. Let $\boldsymbol{P}_A = \boldsymbol{A}^{-1}$, $\boldsymbol{P}_B = \boldsymbol{B}^{-1}$:

$$(\mathbf{x}-\mathbf{a})^\top \boldsymbol{P}_A(\mathbf{x}-\mathbf{a}) + (\mathbf{x}-\mathbf{b})^\top \boldsymbol{P}_B(\mathbf{x}-\mathbf{b})$$
$$= \mathbf{x}^\top(\boldsymbol{P}_A + \boldsymbol{P}_B)\mathbf{x} - 2\mathbf{x}^\top(\boldsymbol{P}_A\mathbf{a} + \boldsymbol{P}_B\mathbf{b}) + \mathbf{a}^\top \boldsymbol{P}_A\mathbf{a} + \mathbf{b}^\top \boldsymbol{P}_B\mathbf{b}.$$

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- Define

$$\boldsymbol{P} := \boldsymbol{P}_A + \boldsymbol{P}_B = \boldsymbol{A}^{-1} + \boldsymbol{B}^{-1}, \quad \boldsymbol{S} := \boldsymbol{P}^{-1}, \quad \mathbf{h} := \boldsymbol{P}_A\mathbf{a} + \boldsymbol{P}_B\mathbf{b}.$$

- We complete the square by choosing m such that $Pm = h$:

$$\mathbf{m} = \boldsymbol{P}^{-1}\mathbf{h} = \boldsymbol{S}(\boldsymbol{A}^{-1}\mathbf{a} + \boldsymbol{B}^{-1}\mathbf{b}).$$

  Then

$$\mathbf{x}^\top\boldsymbol{P}\mathbf{x} - 2\mathbf{x}^\top\mathbf{h} = (\mathbf{x}-\mathbf{m})^\top P(\mathbf{x}-\mathbf{m}) - \mathbf{m}^\top\boldsymbol{P}\mathbf{m}.$$

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- Hence

$$\begin{aligned}\mathcal{N}(\mathbf{x} \mid \mathbf{a}, \boldsymbol{A})\,\mathcal{N}(\mathbf{x} \mid \mathbf{b}, \boldsymbol{B}) &= C_0 \exp\!\left(-\tfrac{1}{2}(\mathbf{x}-\mathbf{m})^\top\boldsymbol{P}(\mathbf{x}-\mathbf{m})\right) \\ &\quad \cdot \exp\!\left(-\tfrac{1}{2}\left[\mathbf{a}^\top\boldsymbol{P}_A\mathbf{a} + \mathbf{b}^\top\boldsymbol{P}_B\mathbf{b} - \mathbf{m}^\top\boldsymbol{P}\mathbf{m}\right]\right),\end{aligned}$$

Proof Step 1: Identifying $\mathcal{N}(\mathbf{x} \mid \mathbf{m}, \boldsymbol{S})$

- Using $\boldsymbol{P} = \boldsymbol{S}^{-1}$, we recognize a Gaussian in $\mathbf{x}$:

$$\exp\big(-\tfrac{1}{2}(\mathbf{x}-\mathbf{m})^\top \boldsymbol{P}(\mathbf{x}-\mathbf{m})\big) = (2\pi)^{D/2}\det(\boldsymbol{S})^{1/2}\,\mathcal{N}(\mathbf{x} \mid \mathbf{m}, \boldsymbol{S}).$$

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- Therefore

$$\mathcal{N}(\mathbf{x} \mid \mathbf{a}, \boldsymbol{A})\,\mathcal{N}(\mathbf{x} \mid \mathbf{b}, \boldsymbol{B}) = \rho\,\mathcal{N}(\mathbf{x} \mid \mathbf{m}, \boldsymbol{S}),$$

  where

$$\begin{aligned}\rho = {} & (2\pi)^{-D/2}\det(\boldsymbol{A})^{-1/2}\det(\boldsymbol{B})^{-1/2}\det(\boldsymbol{S})^{1/2} \\ & \times \exp\Big(-\tfrac{1}{2}\big[\mathbf{a}^\top \boldsymbol{A}^{-1}\mathbf{a} + \mathbf{b}^\top \boldsymbol{B}^{-1}\mathbf{b} - \mathbf{m}^\top \boldsymbol{S}^{-1}\mathbf{m}\big]\Big),\end{aligned}$$

  and we have already identified

$$\boldsymbol{S} = (\boldsymbol{A}^{-1} + \boldsymbol{B}^{-1})^{-1}, \qquad \mathbf{m} = \boldsymbol{S}(\boldsymbol{A}^{-1}\mathbf{a} + \boldsymbol{B}^{-1}\mathbf{b}).$$

- It remains to show that this ρ is equal to $\mathcal{N}(\mathbf{a} \mid \mathbf{b}, \boldsymbol{A}+\boldsymbol{B})$.

Proof Step 2: Determining the Constant ρ (1/2)

- Integrate both sides over $\mathbf{x}$:

$$\int \mathcal{N}(\mathbf{x} \mid \mathbf{a}, \boldsymbol{A})\mathcal{N}(\mathbf{x} \mid \mathbf{b}, \boldsymbol{B})\,\mathrm{d}\mathbf{x} = \rho \int \mathcal{N}(\mathbf{x} \mid \mathbf{m}, \boldsymbol{S})\,\mathrm{d}x = \rho,$$

since $\mathcal{N}(\mathbf{x} \mid \mathbf{m}, \boldsymbol{S})$ is normalized.

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- Give a probabilistic interpretation. Let

$$\boldsymbol{X} \sim \mathcal{N}(\mathbf{b}, \boldsymbol{B}), \qquad \mathbf{a} = \boldsymbol{X} + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \boldsymbol{A}),$$

with $\boldsymbol{X}$ and ε independent.

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  with $\boldsymbol{X}$ and ε independent.

- The joint density of $(\boldsymbol{X}, \mathbf{a})$ is

$$p(\boldsymbol{X}, \mathbf{a}) = p(\mathbf{a} \mid \boldsymbol{X})\,p(\boldsymbol{X}) = \mathcal{N}(\mathbf{a} \mid \boldsymbol{X}, \boldsymbol{A})\,\mathcal{N}(\boldsymbol{X} \mid \mathbf{b}, \boldsymbol{B}).$$

  As a function of $\boldsymbol{X}$, this is precisely $\mathcal{N}(\boldsymbol{X} \mid \mathbf{a}, \boldsymbol{A})\,\mathcal{N}(\boldsymbol{X} \mid \mathbf{b}, \boldsymbol{B})$.

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  As a function of $\boldsymbol{X}$, this is precisely $\mathcal{N}(\boldsymbol{X} \mid \mathbf{a}, \boldsymbol{A})\, \mathcal{N}(\boldsymbol{X} \mid \mathbf{b}, \boldsymbol{B})$.
- The marginal density of $\mathbf{a}$ is Gaussian with mean $\mathbf{b}$ and covariance $\boldsymbol{A} + \boldsymbol{B}$:

$$\mathbf{a} \sim \mathcal{N}(\mathbf{b}, \boldsymbol{A} + \boldsymbol{B}) \quad \Rightarrow \quad p(\mathbf{a}) = \mathcal{N}(\mathbf{a} \mid \mathbf{b}, \boldsymbol{A} + \boldsymbol{B}).$$

Proof Step 2: Determining the Constant c (2/2)

- But

$$p(\mathbf{a}) = \int p(\boldsymbol{X}, \mathbf{a})\,\mathrm{d}\boldsymbol{X} = \int \mathcal{N}(\mathbf{x} \mid \mathbf{a}, \boldsymbol{A})\,\mathcal{N}(\mathbf{x} \mid \mathbf{b}, \boldsymbol{B})\,\mathrm{d}\mathbf{x}.$$

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- Hence

$$\rho = \mathcal{N}(\mathbf{a} \mid \mathbf{b}, \boldsymbol{A} + \boldsymbol{B}),$$

and, by symmetry in **a** and **b**, also $\rho = \mathcal{N}(\mathbf{b} \mid \mathbf{a}, \boldsymbol{A} + \boldsymbol{B})$.

Outline

Motivation

Consider the following examples.

- Assuming that X is a random variable distributed according to some well-known distribution, then what is the distribution of X^2?
- Assuming that X_1, X_2 are two univariate standard normal distributions, then what is the distribution of $\frac{1}{2}(X_1 + X_2)$?

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Consider the following examples.

- Assuming that X is a random variable distributed according to some well-known distribution, then what is the distribution of X^2?
- Assuming that X_1, X_2 are two univariate standard normal distributions, then what is the distribution of $\frac{1}{2}(X_1 + X_2)$?
- What if the transformation is nonlinear?
  - Closed-form expressions are not readily available.

Straightforward for Discrete Random Variables

Example: Univariate Random Variables

Given

- A discrete random variable X with pmf $\Pr[X = x]$.
- An invertible function $U(x)$.

Consider the transformed random variable $Y := U(X)$ with pmf $\Pr[Y = y]$. Then

$$\begin{aligned} \Pr[Y = y] &= \Pr[U(X) = y] && \text{(transformation of interest)} \\ &= \Pr[X = U^{-1}(y)] && \text{(inverse)} \end{aligned}$$

where we can observe $x = U^{-1}(y)$.

Two Approaches

- So far we considered the discrete case (e.g., $\Pr[X = x]$).
- For continuous distributions, we will consider the two approaches:
  1. Cumulative distribution (Distribution Function Technique).
  2. Change-of-variable.

Outline

1. Gaussian Distribution
   - Marginals and Conditionals of Gaussians
   - Sums and Linear Transformations
   - Product of Gaussian Distributions
2. Change of Variables
   - Distribution Function Technique
   - Change of Variables
3. Case Study: Multivariate Gaussian

Distribution Function Technique

Note: a cdf of X: $F_X(x) = \Pr[X \leq x]$.

Goal: Find the cdf of the random variable $Y := U(X)$

1. Find the cdf
$$F_Y(y) = \Pr[Y \leq y].$$

2. Differentiating $F_Y(y)$ to get the pdf $f_Y(y)$:
$$f_Y(y) = \frac{\mathrm{d}}{\mathrm{d}y} F_Y(y).$$

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Note: The domain of the random variable may have changed!

Example

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Let X be a continuous random variable with pdf $f_X : [0, 1] \to [0, 1]$:

$$f_X(x) = 3x^2.$$

Goal: Find the pdf of $Y = X^2$.

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Goal: Find the pdf of $Y = X^2$.

$$\begin{aligned} F_Y(y) &= \Pr[Y \le y] = \Pr[X^2 \le y] \\ &= \Pr[X \le y^{\frac{1}{2}}] \\ &= F_X(y^{\frac{1}{2}}) \end{aligned}$$

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$$\begin{aligned}
F_Y(y) &= \Pr[Y \le y] = \Pr[X^2 \le y] \\
&= \Pr[X \le y^{\frac{1}{2}}] \\
&= F_X(y^{\frac{1}{2}}) = \int_0^{y^{\frac{1}{2}}} 3t^2 \mathrm{d}t \\
&= [t^3]_0^{y^{\frac{1}{2}}} = y^{\frac{3}{2}}, \quad 0 \le y \le 1.
\end{aligned}$$

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Thus,

$$f_Y(y) = \frac{\mathrm{d}}{\mathrm{d}y} F_Y(y) = \frac{3}{2} y^{\frac{1}{2}}$$

for $0 \le y \le 1$.

Exercise

Theorem [Casella & Berger (2002)]

Let X be a continuous random variable with a *strictly monotone* cumulative distribution function $F_X(x)$. Then, the random variable Y defined as

$$Y := F_X(X)$$

has a uniform distribution.

Exercise

Consider $f_X(x) = 3x^2$ in the previous example. Show that $Y := F_X(X)$ attains a uniform distribution.

Remark

The first approach relies on the following facts:

- We can transform the cdf of Y into an expression that is a cdf of X.
- We can differentiate the cdf to obtain the pdf.

Outline

What We have Learnt From the Calculus Course

$$\int f(g(x))g'(x)\mathrm{d}x = \int f(u)\mathrm{d}u, \text{ where } u = g(x).$$

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$$\int f(g(x))g'(x)\mathrm{d}x = \int f(u)\mathrm{d}u, \text{ where } u = g(x).$$

- Intuitively, considering $\mathrm{d}u \approx \Delta u = g'(x)\Delta x$ as the "small changes".

The Roadmap (1/2)

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- Assume that X has states $x \in [a, b]$.
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If U is *strictly increasing*, then so is its inverse U^{-1}.

$$\Pr[U(X) \leq y] = \Pr[U^{-1}(U(X)) \leq U^{-1}(y)]$$

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If U is *strictly increasing*, then so is its inverse U^{-1}.

$$\Pr[U(X) \leq y] = \Pr[U^{-1}(U(X)) \leq U^{-1}(y)] = \Pr[X \leq U^{-1}(y)].$$

Then, $\quad F_Y(y) = \Pr[X \leq U^{-1}(y)] = \int_a^{U^{-1}(y)} f_X(x)\mathrm{d}x$

The Roadmap (2/2)

- To obtain the pdf, we differentiate $F_Y(y)$ w.r.t. y:

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- $\int f_X(U^{-1}(y)) {U^{-1}}'(y) \mathrm{d}y = \int f_X(x) \mathrm{d}x$, where $x = U^{-1}(y)$.

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- To obtain the pdf, we differentiate $F_Y(y)$ w.r.t. y:

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  - The integral on the right-hand side is w.r.t. x, but we need an integral w.r.t. y ($\because$ we are differentiating w.r.t. y...)
  - Change-of-variable comes to the rescue!

- $\displaystyle\int f_X(U^{-1}(y)) U^{-1\prime}(y)\mathrm{d}y = \int f_X(x)\mathrm{d}x$, where $x = U^{-1}(y)$.

- Thus,

$$\begin{aligned} f_Y(y) &= \frac{\mathrm{d}}{\mathrm{d}y} \int_a^{U^{-1}(y)} f_X(U^{-1}(y)) U^{-1\prime}(y)\mathrm{d}y \\ &= f_X(U^{-1}(y)) \cdot \left(\frac{\mathrm{d}}{\mathrm{d}y} U^{-1}(y) \right). \end{aligned}$$

Remark

For decreasing functions,

$$f_Y(y) = -f_X(U^{-1}(y)) \cdot \left(\frac{\mathrm{d}}{\mathrm{d}y} U^{-1}(y)\right).$$

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- The term $\left|\frac{\mathrm{d}}{\mathrm{d}y} U^{-1}(y)\right|$ measures how much a unit volume changes when applying U.

The Main Theorem

Theorem [Billingsley (1995)]

Let $f_X(\mathbf{x})$ be the pdf of the multivariate continuous random variable X. If the vector-valued function $\mathbf{y} = U(\mathbf{x})$ is differentiable and invertible for all values within the domain of $\mathbf{x}$, then for corresponding values of $\mathbf{y}$, the pdf of $Y = U(X)$ is given by

$$f_Y(\mathbf{y}) = f_{\mathbf{x}}(U^{-1}(\mathbf{y})) \cdot \left| \det \left(\frac{\partial}{\partial \mathbf{y}} U^{-1}(\mathbf{y}) \right) \right| .$$

Example

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Consider a bivariate random variable X with states $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ and pdf

$$f\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \frac{1}{2\pi} \exp\left(-\frac{1}{2}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\top \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right).$$

Then, consider a matrix $\boldsymbol{A} \in \mathbb{R}^{2\times 2}$ defined as

$$\boldsymbol{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}.$$

Goal: Find the pdf of the random variable Y with states $\mathbf{y} = \boldsymbol{A}\mathbf{x}$.

- $\mathbf{y} = \boldsymbol{A}\mathbf{x}$

- $\mathbf{y} = \boldsymbol{A}\mathbf{x} \implies \mathbf{x} = \boldsymbol{A}^{-1}\mathbf{y}$.

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \boldsymbol{A}^{-1} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

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- The corresponding pdf is given by

$$f(\mathbf{x}) = f(\boldsymbol{A}^{-1}\mathbf{y}) = \frac{1}{2\pi} \exp\left(-\frac{1}{2}\mathbf{y}^\top (\boldsymbol{A}^{-1})^\top \boldsymbol{A}^{-1}\mathbf{y}\right)$$

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- Thus, $f_Y(\mathbf{y}) = \frac{1}{2\pi} \exp\left(-\frac{1}{2}\mathbf{y}^\top (\boldsymbol{A}^{-1})^\top \boldsymbol{A}^{-1}\mathbf{y}\right) \cdot \left|\frac{1}{ad - bc}\right|$.

Outline

Standard Multivariate Gaussian

- Let $Z = (Z_1, \dots, Z_D)^\top$ with independent coordinates
$$Z_i \sim \mathcal{N}(0,1), \quad i = 1, 2, \dots, D.$$
- The 1D standard Gaussian pdf is
$$\phi(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2}.$$

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$$\phi(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2}.$$
- By independence, the joint density of Z is
$$p_Z(z_1, \ldots, z_D) = \prod_{i=1}^{D} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z_i^2}{2}\right) = (2\pi)^{-D/2} \exp\left(-\frac{1}{2}\sum_{i=1}^{D} z_i^2\right).$$

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Writing $\sum_{i=1}^{D} z_i^2 = \|\mathbf{z}\|^2 = \mathbf{z}^\top \mathbf{z}$, we get

$$p_Z(\mathbf{z}) = (2\pi)^{-D/2} \exp\left(-\frac{1}{2}\mathbf{z}^\top \mathbf{z}\right), \quad \mathbf{z} \in \mathbb{R}^D.$$

Introducing Mean and Covariance

- Let $\boldsymbol{\Sigma}$ be a symmetric positive definite $D \times D$ matrix. Then there exists an invertible L such that

$$\boldsymbol{\Sigma} = LL^\top \quad \text{(e.g. Cholesky factorization).}$$

- Define $X = \boldsymbol{\mu} + LZ$. Then

$$\mathbb{E}[X] = \boldsymbol{\mu} + L\,\mathbb{E}[Z] = \boldsymbol{\mu}, \quad \text{and}$$

$$\begin{aligned} \mathrm{Cov}(X) &= \mathbb{E}[(X-\boldsymbol{\mu})(X-\boldsymbol{\mu})^\top] = \mathbb{E}[LZZ^\top L^\top] \\ &= L\,\mathbb{E}[ZZ^\top]\,L^\top = LI_D L^\top = \boldsymbol{\Sigma}. \end{aligned}$$

- Hence X has mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$; we write $X \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

Change of Variables (1/2)

- The map from Z to X is affine:

$$T(\mathbf{z}) = \boldsymbol{\mu} + L\mathbf{z}, \qquad X = T(Z).$$

Its inverse is

$$z = T^{-1}(\mathbf{x}) = L^{-1}(\mathbf{x} - \boldsymbol{\mu}).$$

- The Jacobian of T^{-1} $\left(\text{i.e., } \frac{\partial}{\partial \mathbf{x}} T^{-1}(\mathbf{x})\right)$ is $J = L^{-1}$, so

$$|\det(J)| = \left|\det(L^{-1})\right| = (\det(L))^{-1}.$$

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- By the change-of-variables formula,

$$p_X(\mathbf{x}) = p_Z\!\left(T^{-1}(\mathbf{x})\right) \left|\det(J)\right|.$$

Change of Variables (2/2)

- From

$$p_X(\mathbf{x}) = p_Z\big(T^{-1}(\mathbf{x})\big)\,\big|\det(J)\big|,$$

Plugging in p_Z and $\mathbf{z} = L^{-1}(\mathbf{x} - \boldsymbol{\mu})$, we obtain

$$\begin{aligned} p_X(\mathbf{x}) &= (2\pi)^{-D/2} \exp\left(-\frac{1}{2}\mathbf{z}^\top \mathbf{z}\right) (\det(L))^{-1} \\ &= (2\pi)^{-D/2} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top (L^{-1})^\top L^{-1} (\mathbf{x} - \boldsymbol{\mu})\right) (\det(L))^{-1}. \end{aligned}$$

Final Form of the Multivariate Gaussian

- Recall that $(L^{-1})^\top L^{-1} = (LL^\top)^{-1} = \mathbf{\Sigma}^{-1}$, and

$$\det(\mathbf{\Sigma}) = \det(LL^\top) = (\det(L))^2 \implies (\det(L))^{-1} = (\det(\mathbf{\Sigma}))^{-1/2}.$$

- Substituting into the previous expression gives

$$p_X(\mathbf{x}) = (2\pi)^{-D/2}(\det(\mathbf{\Sigma}))^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right).$$

- Thus the pdf of the multivariate Gaussian $X \sim \mathcal{N}(\mu, \mathbf{\Sigma})$ is

$$p(\mathbf{x} \mid \boldsymbol{\mu}, \mathbf{\Sigma}) = (2\pi)^{-D/2} \det(\mathbf{\Sigma})^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right).$$

Discussions