

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

1 Gaussian Distribution

- Marginals and Conditionals of Gaussians
- Sums and Linear Transformations

2 Change of Variables

- Distribution Function Technique
- Change of Variables

3 Case Study: Multivariate Gaussian

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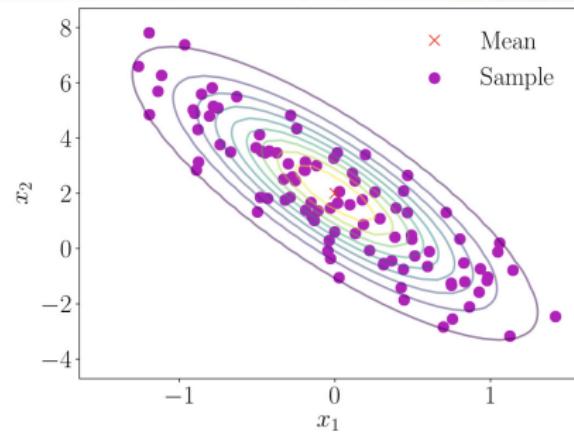
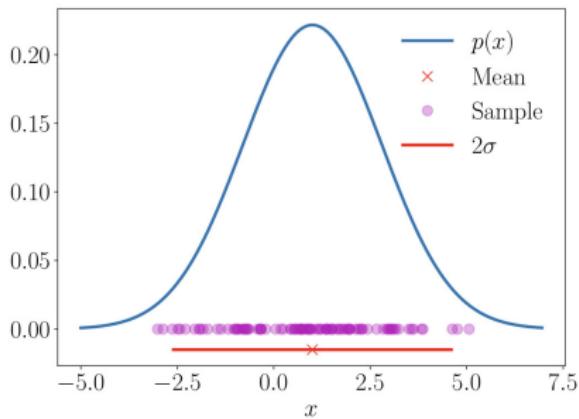
- Distribution Function Technique
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3 Case Study: Multivariate Gaussian

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

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

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

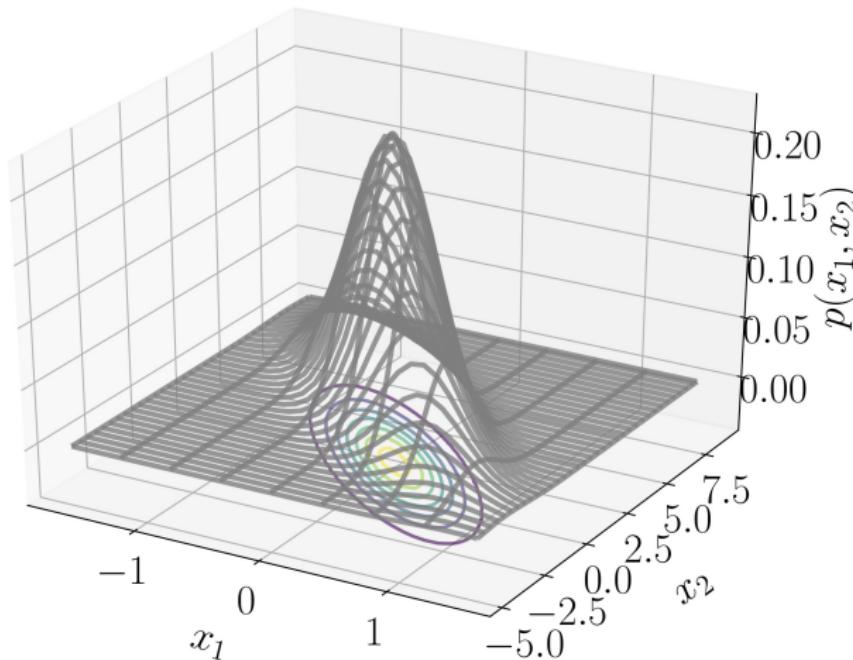
Multivariate

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

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

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

Gaussian distribution of two random variables x_1, x_2 .



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Marginals and Conditionals of Gaussians

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

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

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

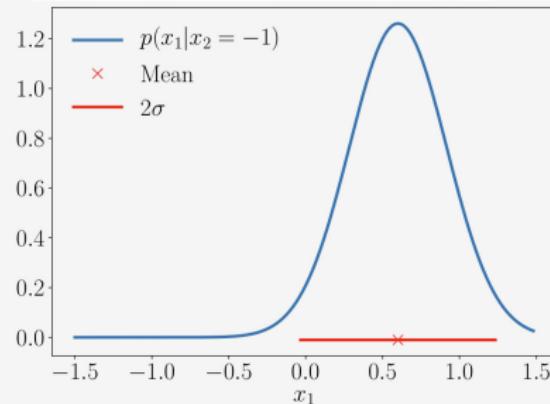
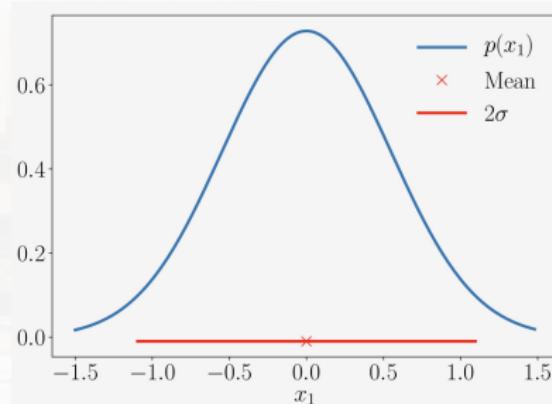
- By [Bishop 2006], the conditional distribution $p(\mathbf{x} | \mathbf{y})$ is also Gaussian.

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

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

Example

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

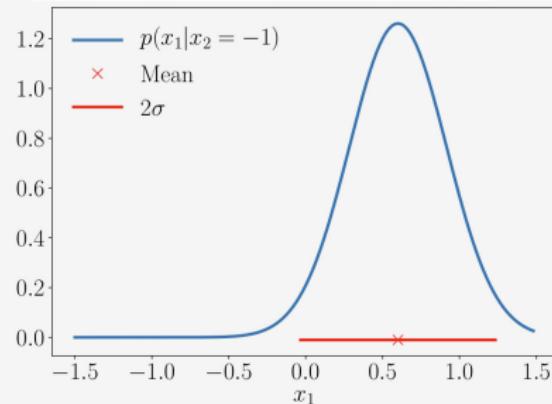
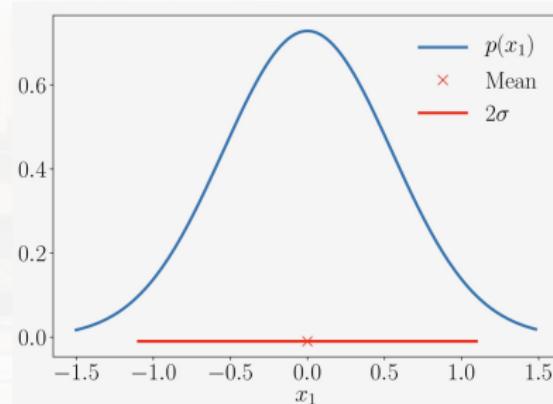


Gaussian Distribution

Marginals and Conditionals of Gaussians

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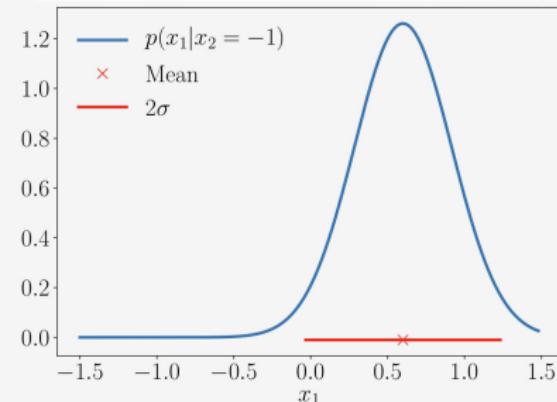
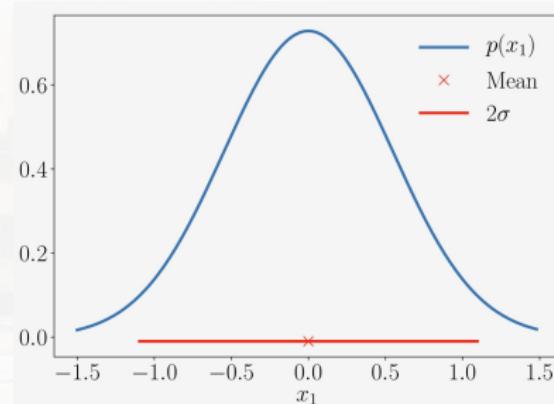
Conditioned on $x_2 = -1$, $\mu_{x_1|x_2=-1} = 0 + (-1) \cdot 0.2 \cdot (-1 - 2) = 0.6$

Gaussian Distribution

Marginals and Conditionals of Gaussians

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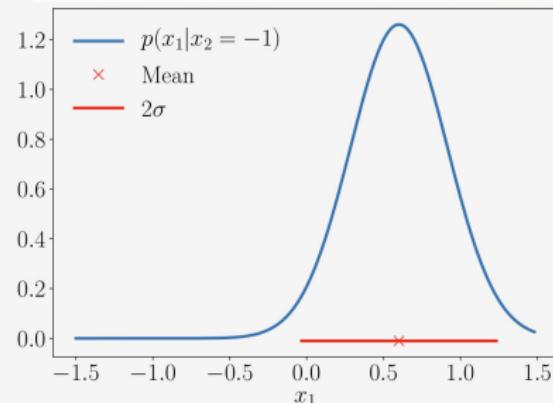
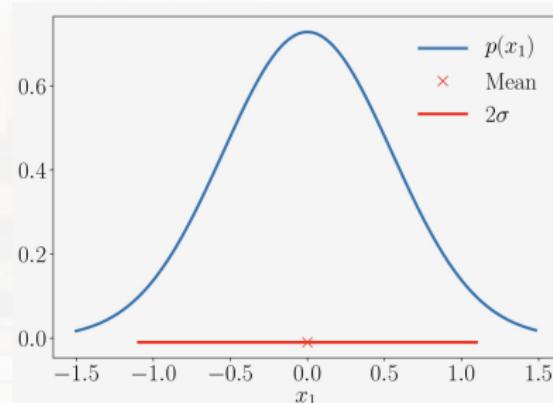
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 and $\sigma_{x_1|x_2=-1}^2 =$

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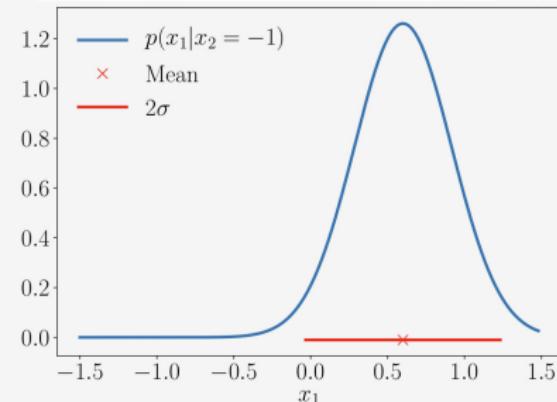
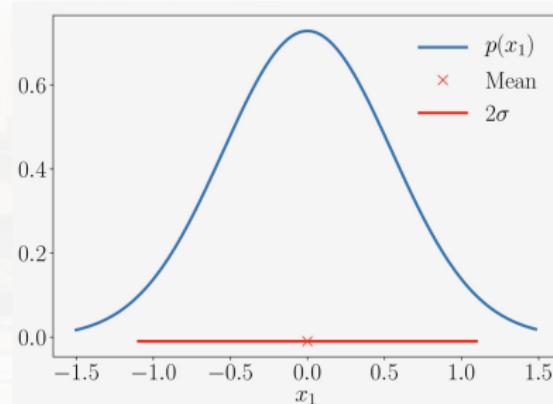


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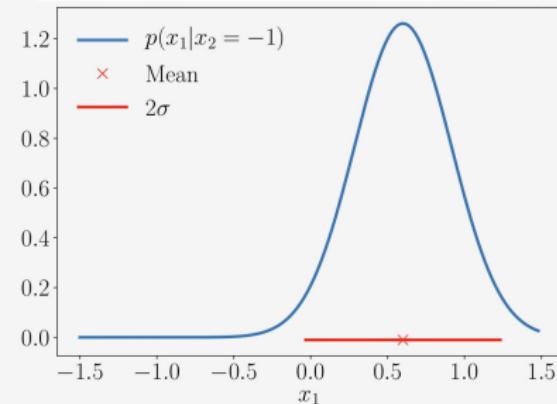
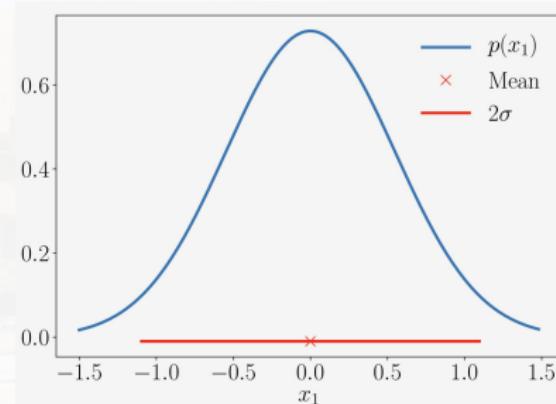


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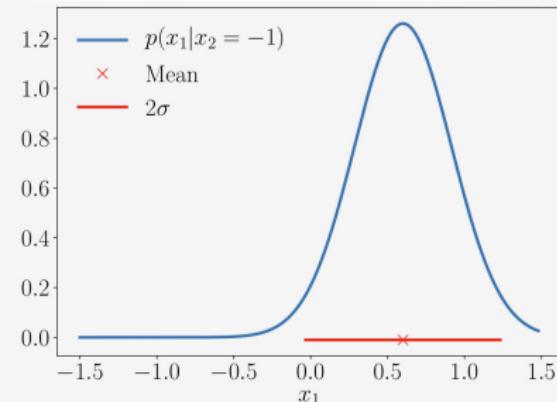
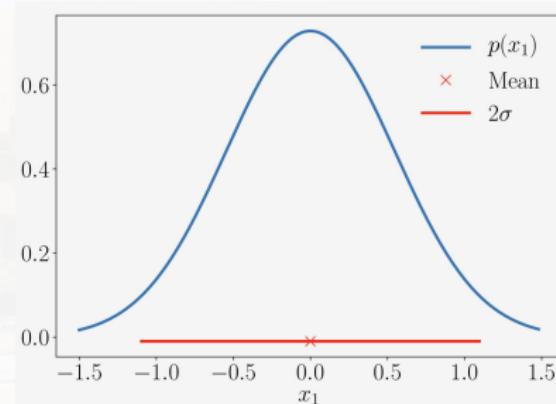


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Sum of Gaussians

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

$$X + Y \sim \mathcal{N}(\mu_x + \mu_y, \Sigma_x + \Sigma_y)$$

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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

$$p(ax + by) =$$

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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,

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

Proof of the Theorem

Sketch:

$$\begin{aligned} \textcircled{1} \quad \mathbb{E}[x] &= \int_{-\infty}^{\infty} xp(x)dx = \int_{-\infty}^{\infty} (\alpha xp_1(x) + (1 - \alpha)xp_2(x))dx \\ &= \alpha\mu_1 + (1 - \alpha)\mu_2. \\ \textcircled{2} \quad \mathbb{E}[x^2] &= \end{aligned}$$

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$$\begin{aligned} \textcircled{2} \quad \mathbb{E}[x^2] &= \int_{-\infty}^{\infty} x^2 p(x)dx = \int_{-\infty}^{\infty} (\alpha x^2 p_1(x) + (1 - \alpha)x^2 p_2(x))dx \\ &= \alpha(\mu_1^2 + \sigma_1^2) + (1 - \alpha)(\mu_2^2 + \sigma_2^2). \end{aligned}$$

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

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Using $\textcircled{1}$ & $\textcircled{2}$ we can prove the theorem.

Linear Transformation by a Matrix (1/2)

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

- The expectation: $\mathbb{E}[\mathbf{y}] = \mathbb{E}[\mathbf{Ax}] =$

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

Linear Transformation by a Matrix (2/2)

Let's consider the **reverse transformation**.

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

- $p(\mathbf{y}) = \mathcal{N}(\mathbf{y} | \mathbf{Ax}, \boldsymbol{\Sigma})$.
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- $y = Ax \iff A^\top y = A^\top Ax \iff (A^\top A)^{-1} A^\top y = x$.
 - This works even for non-invertible A !.
- The variance: $\mathbb{V}[x] = \mathbb{V}[(A^\top A)^{-1} A^\top y] = (A^\top A)^{-1} A^\top \Sigma A (A^\top A)^{-1}$.
- Thus, we have

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

Exercise

Another example of *reverse transformation*.

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

- $p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid \mathbf{Ax}, \Sigma)$.
- 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 $\mathcal{N}(\mu, \Sigma)$.

- However, we only have a sampler of $\mathcal{N}(\mathbf{0}, \mathbf{I})$ at hand.

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- Then, define $\mathbf{y} = \mathbf{A}\mathbf{x} + \mu$, where $\mathbf{A}\mathbf{I}\mathbf{A}^\top = \mathbf{A}\mathbf{A}^\top = \Sigma$.

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

Outline

1 Gaussian Distribution

- Marginals and Conditionals of Gaussians
- Sums and Linear Transformations

2 Change of Variables

- Distribution Function Technique
- Change of Variables

3 Case Study: Multivariate Gaussian

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

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

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.

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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 $f_Y(y)$:

$$f_Y(y) = \frac{d}{dy} F_Y(y).$$

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

Example

Example

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

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

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

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

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

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$$F_Y(y) = \Pr[Y \leq y] = \Pr[X^2 \leq y] \quad \text{Thus,}$$

$$= \Pr[X \leq y^{\frac{1}{2}}] \quad f_Y(y) = \frac{d}{dy} F_Y(y) = \frac{3}{2} y^{\frac{1}{2}}$$

$$= F_X(y^{\frac{1}{2}}) = \int_0^{y^{\frac{1}{2}}} 3t^2 dt \quad \text{for } 0 \leq y \leq 1.$$

$$= [t^3]_0^{y^{\frac{1}{2}}} = y^{\frac{3}{2}}, \quad 0 \leq y \leq 1.$$

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.

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

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

- Intuitively, considering $du \approx \Delta u = g'(x)\Delta x$ as the “small changes”.

The Roadmap (1/2)

- Consider a univariate random variable X and an invertible function U such that $Y := U(X)$.
- Assume that X has states $x \in [a, b]$.
- By the definition of a cdf, we have

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

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

The Roadmap (2/2)

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

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 - $\int f_X(U^{-1}(y)) U^{-1}'(y) dy = \int f_X(x) dx$, where $x = U^{-1}(y)$.
 - Thus,
- $$\begin{aligned} f_Y(y) &= \frac{d}{dy} \int_a^{U^{-1}(y)} f_X(U^{-1}(y)) U^{-1}'(y) dy \\ &= f_X(U^{-1}(y)) \cdot \left(\frac{d}{dy} U^{-1}(y) \right). \end{aligned}$$

Remark

For decreasing functions,

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

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- The term $\left| \frac{d}{dy} U^{-1}(y) \right|$ 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

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

Example

Example

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 $\mathbf{A} \in \mathbb{R}^{2 \times 2}$ defined as

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

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

Change of Variables

Change of Variables

- $\mathbf{y} = \mathbf{Ax}$

Change of Variables

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

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

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

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \mathbf{A}^{-1} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}.$$

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

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

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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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- By independence, the joint density of Z is

$$p_Z(z_1, \dots, z_D) = \prod_{i=1}^D \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z_i^2}{2}\right) = (2\pi)^{-D/2} \exp\left(-\frac{1}{2} \sum_{i=1}^D z_i^2\right).$$

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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 Σ be a symmetric positive definite $D \times D$ matrix. Then there exists an invertible L such that

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

- Define $X = \mu + LZ$. Then

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

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

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

Change of Variables (1/2)

- The map from Z to X is affine:

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

Its inverse is

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

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

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

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

- By the change-of-variables formula,

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

Change of Variables (2/2)

- From

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

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

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

Final Form of the Multivariate Gaussian

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

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

- Substituting into the previous expression gives

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

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

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

Discussions