

Mathematics for Machine Learning

— Probability & Distributions (Supplementary):

Gaussian Distribution & Change of Variables/Inverse Transform

Joseph Chuang-Chieh Lin

Department of Computer Science & Information Engineering,
Tamkang University

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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 Gaussian Distribution
 - Marginals and Conditionals of Gaussians
 - Sums and Linear Transformations
- 2 Change of Variables
 - Distribution Function Technique
 - Change of Variables

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1 Gaussian Distribution

- Marginals and Conditionals of Gaussians
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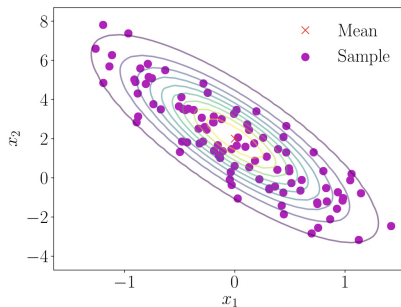
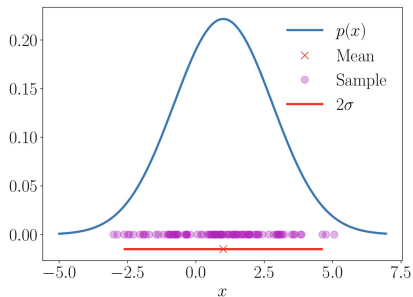
2 Change of Variables

- Distribution Function Technique
- Change of Variables

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

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

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

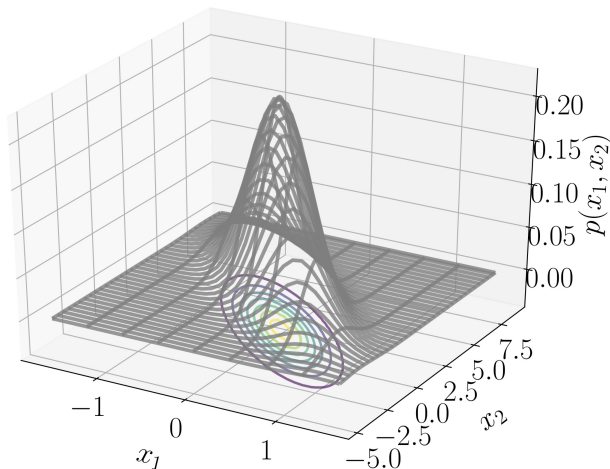
Multivariate

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

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 .



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Marginals and Conditionals of Gaussians

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

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

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

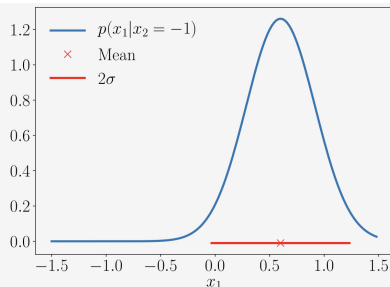
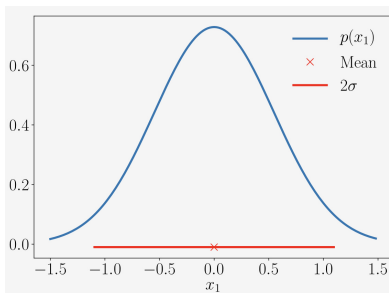
- By [Bishop 2006], the conditional distribution $p(\mathbf{x} | \mathbf{y})$ is also Gaussian.

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

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

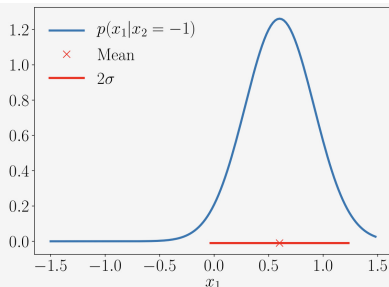
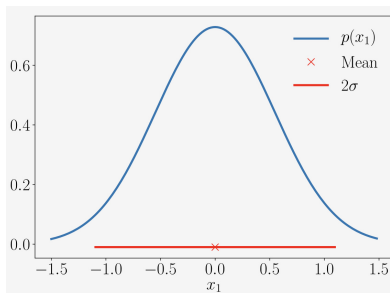
Example

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



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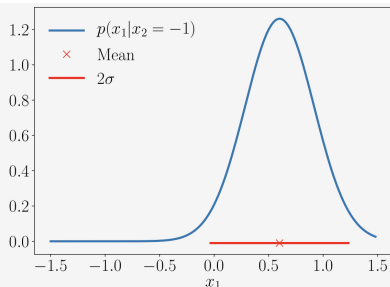
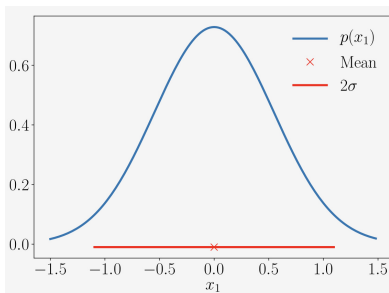
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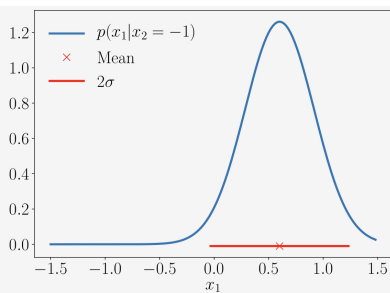
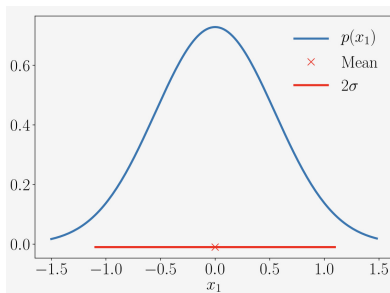
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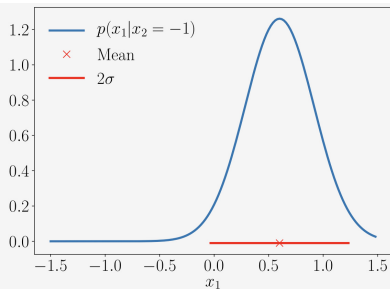
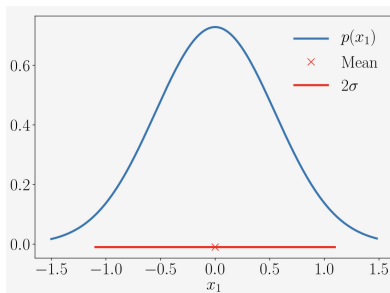


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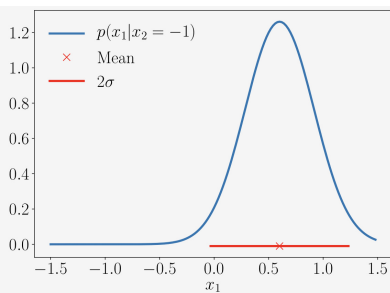
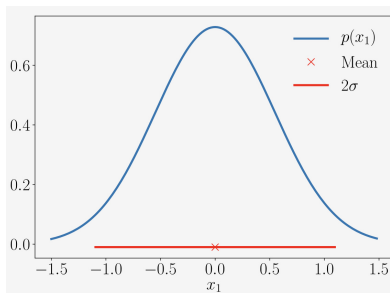


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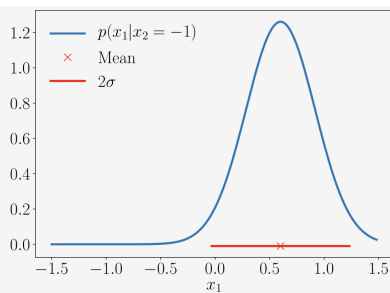
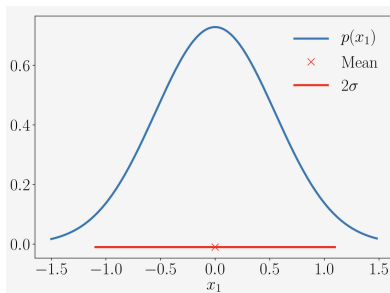


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Sum of Gaussians

Say X, Y are two independent Gaussian random variables with

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

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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 Gaussians

$$p(ax + by) =$$

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$$p(a\mathbf{x} + b\mathbf{y}) = \mathcal{N}(a\mu_x + b\mu_y,$$

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

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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,

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

Proof of the Theorem

Sketch:

$$\textcircled{1} \quad \mathbb{E}[x] = \int_{-\infty}^{\infty} xp(x)dx = \int_{-\infty}^{\infty} (\alpha xp_1(x) + (1 - \alpha)xp_2(x))dx.$$

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

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

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

Linear Transformation by a Matrix (1/2)

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

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

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- Thus, we have

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- The variance: $\mathbb{V}[y] = \mathbb{V}[Ax] = A\mathbb{V}[x]A^\top = A\Sigma A^\top$.
- Thus, we have

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

Linear Transformation by a Matrix (2/2)

Let's consider the *reverse transformation*.

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

- $p(\mathbf{y}) = \mathcal{N}(\mathbf{y} \mid \mathbf{A}\mathbf{x}, \Sigma)$.
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$$X \sim \mathcal{N}((\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mu_y, (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \Sigma \mathbf{A} (\mathbf{A}^\top \mathbf{A})^{-1}).$$

Exercise

Another example of *reverse transformation*.

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

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

A Sampling Approach

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- Then, define $\mathbf{y} = \mathbf{A}\mathbf{x} + \boldsymbol{\mu}$, where $\mathbf{A}\mathbf{A}^\top = \boldsymbol{\Sigma}$.
- To derive \mathbf{A} : Use **Cholesky decomposition** of the covariance matrix $\boldsymbol{\Sigma}$.
 - \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

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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- Assuming that X is a random variable distributed according to some well-known distribution, then **what is the distribution of X^2 ?**
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- 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

- We consider the discrete case (e.g., $\Pr[X = x]$).
- 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 $f_Y(y)$:

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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 $f_X : [0, 1] \mapsto [0, 1]$:

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

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

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

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

The Roadmap (2/2)

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

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- Thus,

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

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

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

Example (On the Backboard)

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 $\mathbf{y} = \mathbf{A}\mathbf{x}$.

Discussions