

Probability Theory Review

STATS 415: Data Mining and Machine Learning

University of Michigan

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The Multivariate Gaussian Distribution

One particularly important example of a probability distribution over random vectors X is called the multivariate Gaussian or multivariate normal distribution. A random vector $X \in \mathbf{R}^d$ is said to have a multivariate normal (or Gaussian) distribution with mean $\mu \in \mathbf{R}^d$ and covariance matrix $\Sigma \in \mathbf{S}_{++}^d$ (where \mathbf{S}_{++}^d refers to the space of symmetric positive definite $d \times d$ matrices)

$$f_{X_1, X_2, \dots, X_d}(x_1, x_2, \dots, x_d; \mu, \Sigma) = \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)\right). \quad (0.1)$$

We write this as $X \sim \mathcal{N}(\mu, \Sigma)$. In this section, we describe multivariate Gaussians and some of their basic properties.

Outline

The Multivariate Gaussian Distribution

Relationship to univariate Gaussians

$$f(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right)$$

The term $(x - \mu)^2$ is a quadratic function. Similarly, $-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)$ is a quadratic form in the vector variable x since Σ is positive definite, i.e.

$$(x - \mu)^T \Sigma^{-1}(x - \mu) > 0$$

The covariance matrix

Proposition: For any random vector X with mean μ and covariance matrix Σ ,

$$\Sigma = E [(X - \mu)(X - \mu)^T] = E [XX^T] - \mu\mu^T$$

The diagonal covariance matrix case

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \quad \Sigma = \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}$$

...

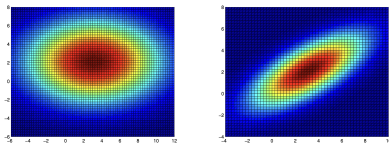
$$f(x; \mu, \Sigma) = \frac{1}{\sqrt{2\pi}\sigma_1} \exp\left(-\frac{1}{2\sigma_1^2} (x_1 - \mu_1)^2\right) \cdot \frac{1}{\sqrt{2\pi}\sigma_2} \exp\left(-\frac{1}{2\sigma_2^2} (x_2 - \mu_2)^2\right)$$

Isocontours

Another way to understand a multivariate Gaussian conceptually is to understand the shape of its isocontours. For a function $f : \mathbf{R}^2 \rightarrow \mathbf{R}$, an isocontour is a set of the form

$$\{x \in \mathbf{R}^2 : f(x) = c\}.$$

for some $c \in \mathbf{R}$



Linear transformation

Theorem: Let $X \sim \mathcal{N}(\mu, \Sigma)$ for some $\mu \in \mathbf{R}^d$ and $\Sigma \in \mathbf{S}_{++}^d$. Then, there exists a matrix $B \in \mathbf{R}^{d \times d}$ such that if we define $Z = B^{-1}(X - \mu)$, then $Z \sim \mathcal{N}(0, I)$

Closure properties

A fancy feature of the multivariate Gaussian distribution is the following set of closure properties:

- ▶ The sum of independent Gaussian random variables is Gaussian.
- ▶ The marginal of a joint Gaussian distribution is Gaussian.
- ▶ The conditional of a joint Gaussian distribution is Gaussian.

Theorem 5.3.: Suppose that $y \sim \mathcal{N}(\mu, \Sigma)$ and $z \sim \mathcal{N}(\mu', \Sigma')$ are independent Gaussian distributed random variables, where $\mu, \mu' \in \mathbf{R}^d$ and $\Sigma, \Sigma' \in \mathbf{S}_{++}^d$. Then, their sum is also Gaussian:

$$y + z \sim \mathcal{N}(\mu + \mu', \Sigma + \Sigma').$$

Closure properties

Suppose that

$$\begin{bmatrix} x_A \\ x_B \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu_A \\ \mu_B \end{bmatrix}, \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix} \right)$$

where $x_A \in \mathbf{R}^n$, $x_B \in \mathbf{R}^d$, and the dimensions of the mean vectors and covariance matrix subblocks are chosen to match x_A and x_B .

Theorem: Then, the marginal densities,

$$p(x_A) = \int_{x_B \in \mathbf{R}^d} p(x_A, x_B; \mu, \Sigma) dx_B$$
$$p(x_B) = \int_{x_A \in \mathbf{R}^n} p(x_A, x_B; \mu, \Sigma) dx_A$$

Closure properties

are Gaussian:

$$x_A \sim \mathcal{N}(\mu_A, \Sigma_{AA})$$

$$x_B \sim \mathcal{N}(\mu_B, \Sigma_{BB}).$$

Closure properties

Theorem: The conditional densities

$$p(x_A | x_B) = \frac{p(x_A, x_B; \mu, \Sigma)}{\int_{x_A \in \mathbf{R}^n} p(x_A, x_B; \mu, \Sigma) dx_A}$$
$$p(x_B | x_A) = \frac{p(x_A, x_B; \mu, \Sigma)}{\int_{x_B \in \mathbf{R}^d} p(x_A, x_B; \mu, \Sigma) dx_B}$$

are also Gaussian:

$$x_A | x_B \sim \mathcal{N}(\mu_A + \Sigma_{AB} \Sigma_{BB}^{-1} (x_B - \mu_B), \Sigma_{AA} - \Sigma_{AB} \Sigma_{BB}^{-1} \Sigma_{BA})$$
$$x_B | x_A \sim \mathcal{N}(\mu_B + \Sigma_{BA} \Sigma_{AA}^{-1} (x_A - \mu_A), \Sigma_{BB} - \Sigma_{BA} \Sigma_{AA}^{-1} \Sigma_{AB})$$