Derivation of Multivariate Normal marginal and conditional distributions

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3 December 2025

Gaussian process regression relies on several special properties of multivariate normal (MVN) distributions. The two most important of those properties are that:

1. The conditional distribution of a multivariate normal is normal
2. The marginal distribution of a multivariate normal is normal

Moreover, these two above items can be calculated in closed form. Suppose that we have an n-dimensional Gaussian[1] random vector[2] $\boldsymbol{x} \in \mathbb{R}^n$. That is,

$$\boldsymbol{x} = \begin{bmatrix} x_1 \sim \mathcal{N}(\mu_1, \sigma_1^2) \\ x_2 \sim \mathcal{N}(\mu_2, \sigma_2^2) \\ \vdots \\ x_n \sim \mathcal{N}(\mu_3, \sigma_3^2) \end{bmatrix}$$

Using vector-matrix notation, we can rewrite the distribution statement as:

$$\boldsymbol{x} \sim \mathcal{N}_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

with the subscipt n indicating that vector $\boldsymbol{x}$ is n-dimensional.

In this case, $\boldsymbol{\mu}$ has become a mean ***vector*** of (possibly different) means for each of our random variables and $\boldsymbol{\Sigma}$ has become a covariace ***matrix***:

[1] Gaussian and normal will be interchanged throughout this document and used as synonyms.

[2] Throughout this document, vectors will be denoted using lowercased bold letters while matrices will be denoted as uppercase bold letters.

$$\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{bmatrix} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1n} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{n1} & \sigma_{n2} & \cdots & \sigma_{nn} \end{bmatrix}$$

We can make a few observations about this formulation:

1. $\boldsymbol{\mu} \in \mathbb{R}^n$ and $\boldsymbol{\Sigma} \in \mathbb{R}^{n \times n}$ (i.e., the mean is n-dimensional and the covariance matrix is $n \times n$-dimensional).
2. $\boldsymbol{\mu}$ is the same number of dimensions as $\boldsymbol{x}$.
3. $\boldsymbol{\mu}$ can assign a different μ_i for each $x_i \in \boldsymbol{x}$.
4. $\boldsymbol{\Sigma}$ is symmetric and all its entries are positive or zero (more strictly, it must be positive semidefinite).
5. The diagnoal of $\boldsymbol{\Sigma}$ is the covariance between x_i and itself, which is the same as the variance of x_i (i.e., $\sigma_{11} = \sigma_1^2$).

The pdf of a multivariate Gaussian is:

$$f(\boldsymbol{x}) = \frac{1}{(2\pi)^{n/2} \det(\boldsymbol{\Sigma})^{1/2}} \exp\left\{\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \boldsymbol{\mu})\right\}$$

Now, let us partition our multivariate normal random vector $\boldsymbol{x} \in \mathbb{R}^n$ into two multvariate normal random vectors $\boldsymbol{x}_a \in \mathbb{R}^d$ and $\boldsymbol{x}_b \in \mathbb{R}^{(n-d)}$:[3]

$$\boldsymbol{x} = \begin{bmatrix} \boldsymbol{x}_a \\ \boldsymbol{x}_b \end{bmatrix}$$

This new partitioned vector should have a multivariate normal distribution denoted by

$$\begin{bmatrix} \boldsymbol{x}_a \\ \boldsymbol{x}_b \end{bmatrix} = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{u}_a \\ \boldsymbol{u}_b \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix}\right)$$

With this background in mind, we can proceed to show that

1. The conditional mean vector and covariance matrix of a multivariate normal for the vector $\boldsymbol{x}_a$ given a realization of the vector $\boldsymbol{x}_b$ are
   - $\boldsymbol{\mu}_{\boldsymbol{x}_a \mid \boldsymbol{x}_b} = \boldsymbol{\mu}_{\boldsymbol{a}} + \boldsymbol{\Sigma}_{ab}\boldsymbol{\Sigma}_{bb}^{-1}(\boldsymbol{x}_b - \boldsymbol{\mu}_b)$
   - $\boldsymbol{\Sigma}_{\boldsymbol{x}_a \mid \boldsymbol{x}_b} = \boldsymbol{\Sigma}_{aa} - \boldsymbol{\Sigma}_{ab}\boldsymbol{\Sigma}_{bb}^{-1}\boldsymbol{\Sigma}_{ba}$

[3]Note the dimensions of each vector!

2. The marginal mean vector and covariance matrix of a multivariate normal for $\boldsymbol{x}_a$ are

   - $\boldsymbol{\mu}_{\boldsymbol{x}_a} = \boldsymbol{\mu}_a$
   - $\boldsymbol{\Sigma}_{\boldsymbol{x}_a} = \boldsymbol{\Sigma}_{aa}$

Let us start with proof of the marginal mean vector and covariance matrix. The marginal pdf of a multivariate