

Derivation of Multivariate Normal marginal and conditional distributions

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1 Background

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 Gaussian¹ random vector² $\mathbf{x} \in \mathbb{R}^n$. That is,

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

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

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

with the subscript n indicating that vector \mathbf{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 covariance **matrix**:

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

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

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

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 \mathbf{x} .
3. $\boldsymbol{\mu}$ can assign a different μ_i for each $x_i \in \mathbf{x}$.
4. $\boldsymbol{\Sigma}$ is symmetric and all its entries are positive or zero (more strictly, it must be positive semidefinite).
5. The diagonal 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:

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

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

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

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

$$\begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix} = \mathcal{N} \left(\begin{bmatrix} \mathbf{u}_a \\ \mathbf{u}_b \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix} \right) \quad (1)$$

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

³Note the dimensions of each vector!

2 Marginal of multivariate normal

Let us start with proof of the marginal mean vector and covariance matrix. The marginal pdf of \mathbf{x}_a is:

$$f(\mathbf{x}_a) = \int_{\mathbb{R}^{(n-d)}} f(\mathbf{x}_a, \mathbf{x}_b) d\mathbf{x}_b$$

because we are integrating out \mathbf{x}_b leaving only the pdf of \mathbf{x}_a . Plugging in the values of the mean vectors and covariance matrices from equation (11), we can write

$$\begin{aligned} f(\mathbf{x}_a) &= \int_{\mathbb{R}^{(n-d)}} \frac{1}{(2\pi)^{n/2} \det(\boldsymbol{\Sigma})^{1/2}} \exp \left\{ -\frac{1}{2} \left(\begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix} - \begin{bmatrix} \mathbf{u}_a \\ \mathbf{u}_b \end{bmatrix} \right)^\top \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix}^{-1} \left(\begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix} - \begin{bmatrix} \mathbf{u}_a \\ \mathbf{u}_b \end{bmatrix} \right) \right\} d\mathbf{x}_b \\ &= \int_{\mathbb{R}^{(n-d)}} \frac{1}{(2\pi)^{n/2} \det(\boldsymbol{\Sigma})^{1/2}} \exp \left\{ -\frac{1}{2} \left(\begin{bmatrix} \mathbf{x}_a - \mathbf{u}_a \\ \mathbf{x}_b - \mathbf{u}_b \end{bmatrix} \right)^\top \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix}^{-1} \left(\begin{bmatrix} \mathbf{x}_a - \mathbf{u}_a \\ \mathbf{x}_b - \mathbf{u}_b \end{bmatrix} \right) \right\} d\mathbf{x}_b \end{aligned}$$

First, to simplify notation, let us define the normalizing constant as

$$Q = (2\pi)^{n/2} \det(\boldsymbol{\Sigma})^{1/2}$$

Now, we need to introduce the concept of the precision matrix $\boldsymbol{\Lambda}$. The precision matrix is defined as the inverse of the covariance matrix: $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$. Using this new definition, we note that

$$\boldsymbol{\Lambda} = \begin{bmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix}^{-1} = \boldsymbol{\Sigma}^{-1}$$

Now we can rewrite the above as:

$$f(\mathbf{x}_a) = \int_{\mathbb{R}^{(n-d)}} \frac{1}{Q} \exp \left\{ -\frac{1}{2} \begin{bmatrix} \mathbf{x}_a - \mathbf{u}_a \\ \mathbf{x}_b - \mathbf{u}_b \end{bmatrix}^\top \begin{bmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{bmatrix} \begin{bmatrix} \mathbf{x}_a - \mathbf{u}_a \\ \mathbf{x}_b - \mathbf{u}_b \end{bmatrix} \right\} d\mathbf{x}_b \quad (2)$$

It is important to note that $\boldsymbol{\Lambda}_{aa} \neq \boldsymbol{\Sigma}_{aa}^{-1}$ but rather that $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$!

Let us expand the positive of the expression within the exponent $\exp\{\cdot\}$ in two steps:

$$\begin{aligned} &\left[\begin{bmatrix} \mathbf{x}_a - \mathbf{u}_a \\ \mathbf{x}_b - \mathbf{u}_b \end{bmatrix}^\top \begin{bmatrix} \boldsymbol{\Lambda}_{aa}(\mathbf{x}_a - \mathbf{u}_a) + \boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \mathbf{u}_b) \\ \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \mathbf{u}_a) + \boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \mathbf{u}_b) \end{bmatrix} \right. \\ &\quad \left. \frac{1}{2} (\mathbf{x}_a - \mathbf{u}_a)^\top \boldsymbol{\Lambda}_{aa} (\mathbf{x}_a - \mathbf{u}_a) + \frac{1}{2} (\mathbf{x}_a - \mathbf{u}_a)^\top \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \mathbf{u}_b) + \right. \\ &\quad \left. + \frac{1}{2} (\mathbf{x}_b - \mathbf{u}_b)^\top \boldsymbol{\Lambda}_{ba} (\mathbf{x}_a - \mathbf{u}_a) + \frac{1}{2} (\mathbf{x}_b - \mathbf{u}_b)^\top \boldsymbol{\Lambda}_{bb} (\mathbf{x}_b - \mathbf{u}_b) \right] \quad (3) \end{aligned}$$

At this point we need to take advantage of the concept of completing the square.

Theorem 1. Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be a symmetric, positive definite matrix and $\{\mathbf{z}, \mathbf{b}, \mathbf{c}\} \in \mathbb{R}^n$, then

$$\frac{1}{2}\mathbf{z}^\top \mathbf{A}\mathbf{z} + \mathbf{b}^\top \mathbf{z} + \mathbf{c} = \frac{1}{2}(\mathbf{z} + \mathbf{A}^{-1}\mathbf{b})^\top \mathbf{A}(\mathbf{z} + \mathbf{A}^{-1}\mathbf{b}) + \mathbf{c} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$$

Lemma 2. Note that $\mathbf{b}^\top \mathbf{z}$ is a scalar ($\mathbb{R}^{1 \times n} \cdot \mathbb{R}^{n \times 1} = 1 \times 1$). Note also that

$$\begin{aligned} \mathbf{b}^\top \mathbf{z} &= [b_1 \ b_2 \ \dots \ b_n] \begin{bmatrix} z_1 \\ z_2 \\ \dots \\ z_n \end{bmatrix} & \mathbf{z}^\top \mathbf{b} &= [z_1 \ z_2 \ \dots \ z_n] \begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_n \end{bmatrix} \\ &= b_1 z_1 + b_2 z_2 + \dots + b_n z_n & &= z_1 b_1 + z_2 b_2 + \dots + z_n b_n \end{aligned}$$

By the commutative property of multiplication of scalars, $\mathbf{b}^\top \mathbf{z} = \mathbf{z}^\top \mathbf{b}$.

Proof. Thus,

$$\frac{1}{2}\mathbf{z}^\top \mathbf{A}\mathbf{z} + \mathbf{b}^\top \mathbf{z} + \mathbf{c} = \frac{1}{2}\mathbf{z}^\top \mathbf{A}\mathbf{z} + \underbrace{\frac{1}{2}\mathbf{b}^\top \mathbf{z} + \frac{1}{2}\mathbf{z}^\top \mathbf{b} + \mathbf{c}}_{\text{from lemma}}$$

Then, add and subtract $\frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$

$$= \frac{1}{2}\mathbf{z}^\top \mathbf{A}\mathbf{z} + \frac{1}{2}\mathbf{b}^\top \mathbf{z} + \frac{1}{2}\mathbf{z}^\top \mathbf{b} + \mathbf{c} + \left(\frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b} \right)$$

Rearrange terms.

$$= \frac{1}{2}\mathbf{b}^\top \mathbf{z} + \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b} + \frac{1}{2}\mathbf{z}^\top \mathbf{A}\mathbf{z} + \frac{1}{2}\mathbf{z}^\top \mathbf{b} + \mathbf{c} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$$

Pull out the $\frac{1}{2}$.

$$= \frac{1}{2}(\mathbf{b}^\top \mathbf{z} + \mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b} + \mathbf{z}^\top \mathbf{A}\mathbf{z} + \mathbf{z}^\top \mathbf{b}) + \mathbf{c} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$$

Rearrange terms.

$$= \frac{1}{2}(\mathbf{z}^\top \mathbf{A}\mathbf{z} + \mathbf{b}^\top \mathbf{z} + \mathbf{z}^\top \mathbf{b} + \mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}) + \mathbf{c} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$$

We can now make a comparison to the scalar version of completing the square:

$$= \frac{1}{2}(\underbrace{\mathbf{z}^\top \mathbf{A}\mathbf{z}}_{\text{like } Ax^2} + \underbrace{\mathbf{b}^\top \mathbf{z} + \mathbf{z}^\top \mathbf{b}}_{\text{like } 2zb} + \underbrace{\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}}_{\text{like } \frac{1}{A}b^2}) + \mathbf{c} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$$

In order to factorize the above in parentheses, we need to fill in some blanks:

$$\frac{1}{2}(\mathbf{z}^\top \mathbf{A}\mathbf{z} + \mathbf{b}^\top \underline{\quad} \mathbf{z} + \mathbf{z}^\top \underline{\quad} \mathbf{b} + \mathbf{b}^\top \mathbf{A}^{-1} \underline{\quad} \mathbf{b}) + \mathbf{c} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$$

To leave the equation the same, we multiply by the identity matrix: $\mathbf{I} = \mathbf{A}\mathbf{A}^{-1}$.

$$= \frac{1}{2}(\mathbf{z}^\top \mathbf{A}\mathbf{z} + \mathbf{z}^\top \mathbf{A}\mathbf{A}^{-1}\mathbf{b} + \mathbf{b}^\top \mathbf{A}^{-1}\mathbf{A}\mathbf{z} + \mathbf{b}^\top \mathbf{A}^{-1}\mathbf{A}\mathbf{A}^{-1}\mathbf{b}) + \mathbf{c} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$$

Pull out $(\mathbf{z} + \mathbf{A}^{-1}\mathbf{b})$ on the right.

$$= \frac{1}{2}(\mathbf{z}^\top \mathbf{A} + \mathbf{b}^\top \mathbf{A}^{-1}\mathbf{A})(\mathbf{z} + \mathbf{A}^{-1}\mathbf{b}) + \mathbf{c} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$$

Pull out \mathbf{A} from the first expression.

$$= \frac{1}{2}(\mathbf{z}^\top + \mathbf{b}^\top \mathbf{A}^{-1})\mathbf{A}(\mathbf{z} + \mathbf{A}^{-1}\mathbf{b}) + \mathbf{c} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$$

Remove a transpose from the first expression.

$$\frac{1}{2}\mathbf{z}^\top \mathbf{A}\mathbf{z} + \mathbf{b}^\top \mathbf{z} + \mathbf{c} = \frac{1}{2}(\mathbf{z} + \mathbf{A}^{-1}\mathbf{b})^\top \mathbf{A}(\mathbf{z} + \mathbf{A}^{-1}\mathbf{b}) + \mathbf{c} - \frac{1}{2}\mathbf{b}^\top \mathbf{A}^{-1}\mathbf{b}$$

□

Back to the problem at hand. Let us complete the square from equation (3):

$$\begin{aligned} & \frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{aa}(\mathbf{x}_a - \boldsymbol{\mu}_a) + \frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b) + \\ & + \frac{1}{2}(\mathbf{x}_b - \boldsymbol{\mu}_b)^\top \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a) + \frac{1}{2}(\mathbf{x}_b - \boldsymbol{\mu}_b)^\top \boldsymbol{\Lambda}_{bb}(\mathbf{x}_b - \boldsymbol{\mu}_b) \end{aligned}$$

Define the following recalling that all precision and covariance matrices are positive semidefinite:

$$\begin{aligned} \mathbf{z} &= \mathbf{x}_b - \boldsymbol{\mu}_b \\ \mathbf{A} &= \boldsymbol{\Lambda}_{bb} & \mathbf{b} &= \boldsymbol{\Lambda}_{ba}(\mathbf{x}_b - \boldsymbol{\mu}_b) \\ \mathbf{c} &= \frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{aa}(\mathbf{x}_a - \boldsymbol{\mu}_a) \end{aligned}$$

Note also that, using the fact that $\boldsymbol{\Lambda}_{ba}^\top = \boldsymbol{\Lambda}_{ab}$,

$$\mathbf{b} = \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a) \implies \mathbf{b}^\top = (\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{ab}$$

We note,

$$\begin{aligned} \frac{1}{2}\mathbf{z}^\top \mathbf{A}\mathbf{z} &= \frac{1}{2}(\mathbf{x}_b - \boldsymbol{\mu}_b)^\top \boldsymbol{\Lambda}_{bb}(\mathbf{x}_b - \boldsymbol{\mu}_b) \\ \mathbf{b}^\top \mathbf{z} &= (\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{ab}(\mathbf{x}_b - \boldsymbol{\mu}_b) \\ \mathbf{c} &= \frac{1}{2}(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{aa}(\mathbf{x}_a - \boldsymbol{\mu}_a) \end{aligned}$$

And applying Theorem (1),

$$\begin{aligned} & \frac{1}{2} \left[((\mathbf{x}_b - \boldsymbol{\mu}_b) + \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a))^{\top} \boldsymbol{\Lambda}_{bb} ((\mathbf{x}_b - \boldsymbol{\mu}_b) + \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a)) \right] \\ & + \frac{1}{2} (\mathbf{x}_a - \boldsymbol{\mu}_a)^{\top} \boldsymbol{\Lambda}_{aa} (\mathbf{x}_a - \boldsymbol{\mu}_a) - \frac{1}{2} (\mathbf{x}_a - \boldsymbol{\mu}_a)^{\top} \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba} (\mathbf{x}_a - \boldsymbol{\mu}_a) \quad (4) \end{aligned}$$

Keeping track of the -1 that we left out when completing the square, and combining (4) with (2), the full expression becomes:

$$\begin{aligned} f(\mathbf{x}_a) = & \frac{1}{Q} \int_{\mathbb{R}^{n-d}} \exp \left\{ -\frac{1}{2} \left[((\mathbf{x}_b - \boldsymbol{\mu}_b) + \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a))^{\top} \boldsymbol{\Lambda}_{bb} ((\mathbf{x}_b - \boldsymbol{\mu}_b) + \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a)) \right] \right. \\ & \left. - \frac{1}{2} (\mathbf{x}_a - \boldsymbol{\mu}_a)^{\top} \boldsymbol{\Lambda}_{aa} (\mathbf{x}_a - \boldsymbol{\mu}_a) + \frac{1}{2} (\mathbf{x}_a - \boldsymbol{\mu}_a)^{\top} \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba} (\mathbf{x}_a - \boldsymbol{\mu}_a) \right\} d\mathbf{x}_b \end{aligned}$$

Since we are integrating over \mathbf{x}_b , all of the terms that contain \mathbf{x}_a can be taken outside of the integral. Using $e^{ab} = e^a e^b$,

$$\begin{aligned} f(\mathbf{x}_a) = & \frac{1}{Q} \exp \left\{ -\frac{1}{2} (\mathbf{x}_a - \boldsymbol{\mu}_a)^{\top} \boldsymbol{\Lambda}_{aa} (\mathbf{x}_a - \boldsymbol{\mu}_a) + \frac{1}{2} (\mathbf{x}_a - \boldsymbol{\mu}_a)^{\top} \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba} (\mathbf{x}_a - \boldsymbol{\mu}_a) \right\} \\ & \int_{\mathbb{R}^{n-d}} \exp \left\{ -\frac{1}{2} \left[((\mathbf{x}_b - \boldsymbol{\mu}_b) + \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a))^{\top} \boldsymbol{\Lambda}_{bb} ((\mathbf{x}_b - \boldsymbol{\mu}_b) + \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a)) \right] \right\} d\mathbf{x}_b \quad (5) \end{aligned}$$

We can remove the inner parentheses $(\mathbf{x}_b - \boldsymbol{\mu}_b) + \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a)$ and instead write $\mathbf{x}_b - \boldsymbol{\mu}_b + \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a)$.

We now observe that if we replace $\boldsymbol{\mu}_b + \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba}(\mathbf{x}_a - \boldsymbol{\mu}_a)$ with \mathbf{m} , the above integral in equation (5) becomes

$$\int_{\mathbb{R}^{n-d}} \exp \left\{ -\frac{1}{2} \left[((\mathbf{x}_b - \mathbf{m})^{\top} \boldsymbol{\Lambda}_{bb} (\mathbf{x}_b - \mathbf{m})) \right] \right\} d\mathbf{x}_b$$

Note, that this integral is a multivariate normal kernel with mean vector \mathbf{m} and covariance matrix $\boldsymbol{\Lambda}_{bb}$ and that we are integrating over the correct dimensionality of \mathbf{x}_b ! Therefore, the integral evaluates to the normalizing constant

$$(2\pi)^{\frac{n-d}{2}} \det(\boldsymbol{\Lambda}_{bb}^{-1})^{1/2}$$

Plugging this into equation (5), we write

$$\begin{aligned} f(\mathbf{x}_a) = & \frac{1}{Q} (2\pi)^{\frac{n-d}{2}} \det(\boldsymbol{\Lambda}_{bb}^{-1})^{1/2} \\ & \exp \left\{ \frac{1}{2} (\mathbf{x}_a - \boldsymbol{\mu}_a)^{\top} \boldsymbol{\Lambda}_{aa} (\mathbf{x}_a - \boldsymbol{\mu}_a) + \frac{1}{2} (\mathbf{x}_a - \boldsymbol{\mu}_a)^{\top} \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba} (\mathbf{x}_a - \boldsymbol{\mu}_a) \right\} \end{aligned}$$

Pulling out a $-\frac{1}{2}$,

$$f(\mathbf{x}_a) = \frac{1}{Q} (2\pi)^{\frac{n-d}{2}} \det(\boldsymbol{\Lambda}_{bb}^{-1})^{1/2} \exp \left\{ -\frac{1}{2} [(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{aa} (\mathbf{x}_a - \boldsymbol{\mu}_a) - (\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba} (\mathbf{x}_a - \boldsymbol{\mu}_a)] \right\}$$

Then pulling out a $(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top$ from the left and an $(\mathbf{x}_a - \boldsymbol{\mu}_a)$ from the right, we get

$$f(\mathbf{x}_a) = \frac{1}{Q} (2\pi)^{n-d/2} \det(\boldsymbol{\Lambda}_{bb}^{-1})^{1/2} \exp \left\{ -\frac{1}{2} [(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \boldsymbol{\Lambda}_{aa} - \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba} (\mathbf{x}_a - \boldsymbol{\mu}_a)] \right\} \quad (6)$$

Equation (6) appears to be a MVN with mean vector $\boldsymbol{\mu}_a$ and covariance matrix $\boldsymbol{\Lambda}_{aa} - \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba}$. Now, all that is left is to rewrite the covariance matrix and the normalization constant in terms of $\boldsymbol{\Sigma}$.

Recall,

$$\boldsymbol{\Lambda} = \begin{bmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix}^{-1} = \boldsymbol{\Sigma}^{-1}$$

Thus, $\boldsymbol{\Lambda}^{-1} = \boldsymbol{\Sigma}$ and

$$\begin{bmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{bmatrix}^{-1} = \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix}$$

We now need a result from linear algebra.

Theorem 3. Let \mathbf{M} be a symmetric, positive definite block matrix,

$$\mathbf{M} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}$$

We can define \mathbf{M}^{-1} using the Shur complement, \mathbf{D} in \mathbf{M} : $(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1}$.

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}^{-1} = \begin{bmatrix} (\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1} & -(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1}\mathbf{B}\mathbf{D}^{-1} \\ -\mathbf{D}\mathbf{C}(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{C}(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1}\mathbf{B}\mathbf{D}^{-1} \end{bmatrix}$$

Using Theorem (3), we write

$$\begin{aligned} \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix} &= \begin{bmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{bmatrix}^{-1} \\ &= \begin{bmatrix} (\boldsymbol{\Lambda}_{aa} - \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba})^{-1} & -(\boldsymbol{\Lambda}_{aa} - \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba})^{-1} \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \\ -\boldsymbol{\Lambda}_{bb} \boldsymbol{\Lambda}_{ba} (\boldsymbol{\Lambda}_{aa} - \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba})^{-1} & \boldsymbol{\Lambda}_{bb}^{-1} + \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba} (\boldsymbol{\Lambda}_{aa} - \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \boldsymbol{\Lambda}_{ba})^{-1} \boldsymbol{\Lambda}_{ab} \boldsymbol{\Lambda}_{bb}^{-1} \end{bmatrix} \end{aligned} \quad (7)$$

Reading across, we see that

$$\begin{aligned}\boldsymbol{\Sigma}_{aa} &= (\boldsymbol{\Lambda}_{aa} - \boldsymbol{\Lambda}_{ab}\boldsymbol{\Lambda}_{bb}^{-1}\boldsymbol{\Lambda}_{ba})^{-1} \\ \boldsymbol{\Sigma}_{aa}^{-1} &= \boldsymbol{\Lambda}_{aa} - \boldsymbol{\Lambda}_{ab}\boldsymbol{\Lambda}_{bb}^{-1}\boldsymbol{\Lambda}_{ba}\end{aligned}$$

Lastly, we handle the normalization constant. We need one more result from linear algebra regarding the determinant of block matrices:

Theorem 4. *Again, let \mathbf{M} be a symmetric, positive definite block matrix,*

$$\mathbf{M} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}$$

The determinant of \mathbf{M} is

$$\det(\mathbf{M}) = \det(\mathbf{A}) \det(\mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B})$$

From equation (6), we pull the constant, and replace Q with its value,

$$\frac{1}{Q}(2\pi)^{\frac{n-d}{2}} \det((\boldsymbol{\Lambda}_{bb}^{-1})^{1/2}) = (2\pi)^{\frac{-n}{2}} \det(\boldsymbol{\Sigma})^{-1/2} (2\pi)^{\frac{n-d}{2}} \det((\boldsymbol{\Lambda}_{bb}^{-1})^{1/2}) \quad (8)$$

Using theorem (4), the determinant of the block matrix $\boldsymbol{\Sigma}$ is

$$\det(\boldsymbol{\Sigma}) = \det(\boldsymbol{\Sigma}_{aa}) \det(\boldsymbol{\Sigma}_{bb} - \boldsymbol{\Sigma}_{ba}\boldsymbol{\Sigma}_{aa}^{-1}\boldsymbol{\Sigma}_{ab})$$

Plugging this into equation (8) and distributing the exponent $-1/2$, we can write,

$$= (2\pi)^{\frac{-n}{2}} \det(\boldsymbol{\Sigma}_{aa})^{-1/2} \det(\boldsymbol{\Sigma}_{bb} - \boldsymbol{\Sigma}_{ba}\boldsymbol{\Sigma}_{aa}^{-1}\boldsymbol{\Sigma}_{ab})^{-1/2} (2\pi)^{\frac{n-d}{2}} \det((\boldsymbol{\Lambda}_{bb}^{-1})^{1/2})$$

Rearranging terms.

$$= (2\pi)^{\frac{-n}{2}} (2\pi)^{\frac{n-d}{2}} \det(\boldsymbol{\Sigma}_{aa})^{-1/2} \det(\boldsymbol{\Sigma}_{bb} - \boldsymbol{\Sigma}_{ba}\boldsymbol{\Sigma}_{aa}^{-1}\boldsymbol{\Sigma}_{ab})^{-1/2} \det((\boldsymbol{\Lambda}_{bb}^{-1})^{1/2})$$

Combining exponents over π .

$$= (2\pi)^{\frac{-d}{2}} \det(\boldsymbol{\Sigma}_{aa})^{-1/2} \det(\boldsymbol{\Sigma}_{bb} - \boldsymbol{\Sigma}_{ba}\boldsymbol{\Sigma}_{aa}^{-1}\boldsymbol{\Sigma}_{ab})^{-1/2} \det((\boldsymbol{\Lambda}_{bb}^{-1})^{1/2})$$

And if

$$\boldsymbol{\Sigma}_{aa} = (\boldsymbol{\Lambda}_{aa} - \boldsymbol{\Lambda}_{ab}\boldsymbol{\Lambda}_{bb}^{-1}\boldsymbol{\Lambda}_{ba})^{-1}$$

then,

$$\boldsymbol{\Sigma}_{bb} = (\boldsymbol{\Lambda}_{bb} - \boldsymbol{\Lambda}_{ba}\boldsymbol{\Lambda}_{aa}^{-1}\boldsymbol{\Lambda}_{ab})^{-1}$$

and likewise

$$\begin{aligned}\boldsymbol{\Lambda}_{bb} &= (\boldsymbol{\Sigma}_{bb} - \boldsymbol{\Sigma}_{ba}\boldsymbol{\Sigma}_{aa}^{-1}\boldsymbol{\Sigma}_{ab})^{-1} \\ \boldsymbol{\Lambda}_{bb}^{-1} &= (\boldsymbol{\Sigma}_{bb} - \boldsymbol{\Sigma}_{ba}\boldsymbol{\Sigma}_{aa}^{-1}\boldsymbol{\Sigma}_{ab})\end{aligned}$$

Replacing the Λ_{bb}^{-1} , we write

$$(2\pi)^{\frac{-d}{2}} \det(\Sigma_{aa})^{-1/2} \det(\Sigma_{bb} - \Sigma_{ba}\Sigma_{aa}^{-1}\Sigma_{ab})^{-1/2} \det(\Sigma_{bb} - \Sigma_{ba}\Sigma_{aa}^{-1}\Sigma_{ab})^{1/2}$$

The two determinants on the right cancel leaving the final normalizing constant as

$$(2\pi)^{\frac{-d}{2}} \det(\Sigma_{aa})^{-1/2}$$

We can now rewrite equation (6) as

$$f(\mathbf{x}_a) = \frac{1}{(2\pi)^{\frac{-d}{2}} \det(\Sigma_{aa})^{-1/2}} \exp \left\{ -\frac{1}{2} \left[(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \underbrace{\Lambda_{aa} - \Lambda_{ab}\Lambda_{bb}^{-1}\Lambda_{ba}}_{\Sigma_{aa}^{-1}} (\mathbf{x}_a - \boldsymbol{\mu}_a) \right] \right\} \quad (9)$$

$$= \frac{1}{(2\pi)^{\frac{d}{2}} \det(\Sigma_{aa})^{1/2}} \exp \left\{ -\frac{1}{2} [(\mathbf{x}_a - \boldsymbol{\mu}_a)^\top \Sigma_{aa}^{-1} (\mathbf{x}_a - \boldsymbol{\mu}_a)] \right\} \quad (10)$$

Recall that we defined \mathbf{x}_a as a multivariate normal random vector in \mathbb{R}^d . Therefore, miraculously, the exponent in the normalizing constant is correct! Furthermore, it is clear that the last equation (10), is the multivariate normal pdf with mean vector $\boldsymbol{\mu}_a$ and covariance matrix Σ_{aa} . Thus,

$$p(\mathbf{x}_a) \sim \mathcal{N}(\boldsymbol{\mu}_a, \Sigma_{aa})$$

and likewise

$$p(\mathbf{x}_b) \sim \mathcal{N}(\boldsymbol{\mu}_b, \Sigma_{bb}) \quad \square$$

3 Conditional of multivariate normal

Remaining in the same setup, our multivariate normal random vector $\mathbf{x} \in \mathbb{R}^n$ has two multivariate normal random vector partitions $\mathbf{x}_a \in \mathbb{R}^d$ and $\mathbf{x}_b \in \mathbb{R}^{(n-d)}$.

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

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

$$\begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix} = \mathcal{N} \left(\begin{bmatrix} \mathbf{u}_a \\ \mathbf{u}_b \end{bmatrix}, \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix} \right) \quad (11)$$

We now are looking to solve for $p(\mathbf{x}_a | \mathbf{x}_b)$. Using Bayes' theorem, we have

$$p(\mathbf{x}_a | \mathbf{x}_b) = \frac{p(\mathbf{x}_a, \mathbf{x}_b)}{p(\mathbf{x}_b)} \propto p(\mathbf{x}_a, \mathbf{x}_b)$$

Using the definition of the pdf of a multivariate normal and the proof of the marginal distribution of a multivariate normal that was just proven, we write,

$$p(\mathbf{x}_a | \mathbf{x}_b) = \frac{\frac{1}{(2\pi)^{\frac{n}{2}} \det(\boldsymbol{\Sigma})^{1/2}} \exp\left\{-\frac{1}{2} [(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})]\right\}}{\frac{1}{(2\pi)^{\frac{n-d}{2}} \det(\boldsymbol{\Sigma}_{bb})^{1/2}} \exp\left\{-\frac{1}{2} [(\mathbf{x}_b - \boldsymbol{\mu}_b)^\top \boldsymbol{\Sigma}_{bb}^{-1} (\mathbf{x}_b - \boldsymbol{\mu}_b)]\right\}}$$

Clean up the fraction and combine the exponents.

$$\begin{aligned} &= \frac{(2\pi)^{\frac{n-d}{2}}}{(2\pi)^{\frac{n}{2}}} \frac{\det(\boldsymbol{\Sigma}_{bb})^{1/2}}{\det(\boldsymbol{\Sigma})^{1/2}} \exp\left\{-\frac{1}{2} [(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})] + \frac{1}{2} [(\mathbf{x}_b - \boldsymbol{\mu}_b)^\top \boldsymbol{\Sigma}_{bb}^{-1} (\mathbf{x}_b - \boldsymbol{\mu}_b)]\right\} \end{aligned}$$

We can use the same method of partitioning as equation (2) to write

$$\begin{aligned} &= \frac{1}{(2\pi)^{\frac{d}{2}}} \frac{\det(\boldsymbol{\Sigma}_{bb})^{1/2}}{\det(\boldsymbol{\Sigma})^{1/2}} \exp\left\{-\frac{1}{2} \begin{bmatrix} \mathbf{x}_a - \mathbf{u}_a \\ \mathbf{x}_b - \mathbf{u}_b \end{bmatrix}^\top \begin{bmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{bmatrix} \begin{bmatrix} \mathbf{x}_a - \mathbf{u}_a \\ \mathbf{x}_b - \mathbf{u}_b \end{bmatrix} + \frac{1}{2} [(\mathbf{x}_b - \boldsymbol{\mu}_b)^\top \boldsymbol{\Sigma}_{bb}^{-1} (\mathbf{x}_b - \boldsymbol{\mu}_b)]\right\} \end{aligned}$$

Removing the normalization constant for ease, and expanding the matrix multiplications as we did above in equation (3),

$$\begin{aligned} &\exp\left\{-\frac{1}{2} ((\mathbf{x}_a - \mathbf{u}_a)^\top \boldsymbol{\Lambda}_{aa} (\mathbf{x}_a - \mathbf{u}_a) + (\mathbf{x}_a - \mathbf{u}_a)^\top \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \mathbf{u}_b) + (\mathbf{x}_b - \mathbf{u}_b)^\top \boldsymbol{\Lambda}_{ba} (\mathbf{x}_a - \mathbf{u}_a) + (\mathbf{x}_b - \mathbf{u}_b)^\top \boldsymbol{\Lambda}_{bb} (\mathbf{x}_b - \mathbf{u}_b) + \frac{1}{2} (\mathbf{x}_b - \boldsymbol{\mu}_b)^\top \boldsymbol{\Sigma}_{bb}^{-1} (\mathbf{x}_b - \boldsymbol{\mu}_b))\right\} \end{aligned}$$