Derivation of Multivariate Normal marginal and conditional distributions

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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

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

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 $\boldsymbol{x}_a$ 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 $\boldsymbol{x}_a$ is:

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

because we are integrating out $\boldsymbol{x}_b$ leaving only the pdf of $\boldsymbol{x}_a$. Plugging in the values of the mean vectors and covariance matrices from equation (1), we can write

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

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:

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

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:

$$\begin{bmatrix} \boldsymbol{x}_a - \boldsymbol{u}_a \\ \boldsymbol{x}_b - \boldsymbol{u}_b \end{bmatrix}^\top \begin{bmatrix} \boldsymbol{\Lambda}_{aa}(\boldsymbol{x}_a - \boldsymbol{u}_a) + \boldsymbol{\Lambda}_{ab}(\boldsymbol{x}_b - \boldsymbol{u}_b) \\ \boldsymbol{\Lambda}_{ba}(\boldsymbol{x}_a - \boldsymbol{u}_a) + \boldsymbol{\Lambda}_{ab}(\boldsymbol{x}_b - \boldsymbol{u}_b) \end{bmatrix}$$

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

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

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

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

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

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

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

Proof. Thus,

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

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

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

Rearrange terms.

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

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

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

Rearrange terms.

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

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

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

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

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

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

$$\begin{aligned}
&= \frac{1}{2}(\boldsymbol{z}^\top \boldsymbol{A}\boldsymbol{z} + \boldsymbol{z}^\top \boldsymbol{A}\boldsymbol{A}^{-1}\boldsymbol{b} + \boldsymbol{b}^\top \boldsymbol{A}^{-1}\boldsymbol{A}\boldsymbol{z} + \boldsymbol{b}^\top \boldsymbol{A}^{-1}\boldsymbol{A}\boldsymbol{A}^{-1}\boldsymbol{b}) + \boldsymbol{c} - \frac{1}{2}\boldsymbol{b}^\top \boldsymbol{A}^{-1}\boldsymbol{b} \\
&\text{Pull out } (\boldsymbol{z} + \boldsymbol{A}^{-1}\boldsymbol{b}) \text{ on the right.} \\
&= \frac{1}{2}(\boldsymbol{z}^\top \boldsymbol{A} + \boldsymbol{b}^\top \boldsymbol{A}^{-1}\boldsymbol{A})(\boldsymbol{z} + \boldsymbol{A}^{-1}\boldsymbol{b}) + \boldsymbol{c} - \frac{1}{2}\boldsymbol{b}^\top \boldsymbol{A}^{-1}\boldsymbol{b} \\
&\text{Pull out } \boldsymbol{A} \text{ from the first expression.} \\
&= \frac{1}{2}(\boldsymbol{z}^\top + \boldsymbol{b}^\top \boldsymbol{A}^{-1})\boldsymbol{A}(\boldsymbol{z} + \boldsymbol{A}^{-1}\boldsymbol{b}) + \boldsymbol{c} - \frac{1}{2}\boldsymbol{b}^\top \boldsymbol{A}^{-1}\boldsymbol{b} \\
&\text{Remove a transpose from the first expression.} \\
\frac{1}{2}\boldsymbol{z}^\top \boldsymbol{A}\boldsymbol{z} + \boldsymbol{b}^\top \boldsymbol{z} + \boldsymbol{c} &= \frac{1}{2}(\boldsymbol{z} + \boldsymbol{A}^{-1}\boldsymbol{b})^\top \boldsymbol{A}(\boldsymbol{z} + \boldsymbol{A}^{-1}\boldsymbol{b}) + \boldsymbol{c} - \frac{1}{2}\boldsymbol{b}^\top \boldsymbol{A}^{-1}\boldsymbol{b}
\end{aligned}$$

□

Back to the problem at hand. Let us complete the square:

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

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

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

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

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

We note,

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

And applying Theorem (1),

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