
Supplementary Materials for Improving Quadrature for Constrained Integrand

1 Derivation of Moments

This section provides the derivation of the first and second raw moments for the log and probit transforms, as shown in Table 1, and the relevant partial derivatives, which are required to use gradient based methods to optimize the GP hyperparameters in f -space as described in the main text.

1.1 Log transform moments

Let $\mathbf{y} = \{y_1, \dots, y_n\}$ be a multivariate Gaussian random variable with mean vector $\boldsymbol{\mu}$ and covariance matrix Σ and let $\mathbf{x} = \exp(\mathbf{y})$. Then \mathbf{x} follows a multivariate log-normal distribution [1, 2, 5], a well-studied distribution whose first and second raw moments are given by

$$\mathbb{E}[x_i] = \exp\left(\mu_i + \frac{\Sigma_{ii}}{2}\right) \quad (1)$$

$$\mathbb{E}[x_i^2] = \exp(2\mu_i + 2\Sigma_{ii}) \quad (2)$$

$$\mathbb{E}[x_i x_j] = \exp\left(\mu_i + \mu_j + \frac{1}{2}(\Sigma_{ii} + \Sigma_{jj}) + \Sigma_{ij}\right), \quad (3)$$

where x_i is the i^{th} element of the vector \mathbf{x} , μ_i is the mean of the i^{th} element of y_i and Σ_{ij} is the covariance between y_i and y_j . The derivation of these moments is omitted as they are well established in the literature and not very interesting (they follow from a simple substitution and then completing the square within the exponent).

In order to fit hyperparameters in f -space as described in the main text, we maximize the likelihood of some observed training dataset (or equivalently, minimize the negative log-likelihood) w.r.t. the hyperparameters of the GP prior on the g -space belief. Making use of equation 5.8 from Rasmussen and Williams [3], it follows that the relevant quantities are $\partial\mathbb{E}[x_i]/\partial\theta$ and $\partial\mathbb{E}[x_i x_j]/\partial\theta$ where θ is some hyperparameter of either the mean or covariance function of the GP prior. Because the partial derivatives $\partial\mu/\partial\theta$ and $\partial\Sigma/\partial\theta$ depend on the choice of mean and covariance function, we instead present the partial derivatives of the moments w.r.t. the means and covariances/variances. These partial derivatives can be used in conjunction with $\partial\mu/\partial\theta$ and $\partial\Sigma/\partial\theta$ to compute the gradient of the negative log-likelihood w.r.t. the g -space GP hyperparameters via the chain rule.

The relevant partial derivatives for the log transform are trivial to compute:

$$\frac{\partial\mathbb{E}[x_i]}{\partial\mu_i} = \exp\left(\mu_i + \frac{\Sigma_{ii}}{2}\right) \quad (4)$$

$$\frac{\partial\mathbb{E}[x_i]}{\partial\Sigma_{ii}} = \frac{1}{2} \exp\left(\mu_i + \frac{\Sigma_{ii}}{2}\right) \quad (5)$$

$$\frac{\partial\mathbb{E}[x_i^2]}{\partial\mu_i} = 2 \exp(2\mu_i + 2\Sigma_{ii}) \quad (6)$$

$$\frac{\partial\mathbb{E}[x_i^2]}{\partial\Sigma_{ii}} = 2 \exp(2\mu_i + 2\Sigma_{ii}) \quad (7)$$

$$\frac{\partial\mathbb{E}[x_i x_j]}{\partial\mu_i} = \exp\left(\mu_i + \mu_j + \frac{1}{2}(\Sigma_{ii} + \Sigma_{jj}) + \Sigma_{ij}\right) \quad (8)$$

$$\frac{\partial\mathbb{E}[x_i x_j]}{\partial\Sigma_{ii}} = \frac{1}{2} \exp\left(\mu_i + \mu_j + \frac{1}{2}(\Sigma_{ii} + \Sigma_{jj}) + \Sigma_{ij}\right) \quad (9)$$

$$\frac{\partial\mathbb{E}[x_i x_j]}{\partial\Sigma_{ij}} = \exp\left(\mu_i + \mu_j + \frac{1}{2}(\Sigma_{ii} + \Sigma_{jj}) + \Sigma_{ij}\right) \quad (10)$$

1.2 Probit transform moments

To derive the first raw moment associated with the probit transform, we take an approach similar to the one found in section 3.9 of Rasmussen and Williams [3]: let $\mathbf{y} = \{y_1, \dots, y_n\}$ be a multivariate Gaussian random variable with mean vector $\boldsymbol{\mu}$ and covariance matrix Σ and let $\mathbf{x} = \Phi(\mathbf{y})$. The first raw moment of x_i is

$$\begin{aligned} \mathbb{E}[x_i] &= \int_{-\infty}^{\infty} \Phi(w) \phi(w, \mu_i, \Sigma_{ii}) dw \quad (11) \\ &= \frac{1}{2\pi\sqrt{\Sigma_{ii}}} \int_{-\infty}^{\infty} \int_{-\infty}^w \exp\left(-\frac{z^2}{2} - \frac{(w - \mu_i)^2}{2\Sigma_{ii}}\right) dz dw. \quad (12) \end{aligned}$$

We make the following substitutions: $a = w - \mu_i$ and $b = z - a$. Plugging these substitutions in and then switching the order of the integrals gives

$$\mathbb{E}[x_i] = \frac{1}{2\pi\sqrt{\Sigma_{ii}}} \int_{-\infty}^{\mu_i} \int_{-\infty}^{\infty} \exp\left(-\frac{(a+b)^2}{2} - \frac{a^2}{2\Sigma_{ii}}\right) da db. \quad (13)$$

Table 1: Induced (*raw*) first and second moments of $f = \xi(g)$ for the log and probit transformations; the covariance function can be computed by $K(x, x') = C(x, x') - m(x)m(x')$. Some entries for the second raw moment refer to values of the first moment for that transform.

transform	first moment $m(x) = \mathbb{E}[f(x)]$	second raw moment $C(x, x') = \mathbb{E}[f(x)f(x')]$
$\xi(f) = \exp(f)$	$\exp(\mu(x) + 1/2\Sigma(x, x))$	$m(x) \exp(\Sigma(x, x')) m(x')$
$\xi(f) = \Phi(f)$	$\Phi\left(\frac{\mu(x)}{\sqrt{\Sigma(x, x) + 1}}\right)$	$\Phi\left(\left[\begin{array}{c} \mu(x) \\ \mu(x') \end{array}\right], \left[\begin{array}{cc} \Sigma(x, x) + 1 & \Sigma(x, x') \\ \Sigma(x', x) & \Sigma(x', x') + 1 \end{array}\right]\right)$

Observe that the quantity inside the exponent of (13) can be written using matrix notation as

$$(a + b)^2 + \frac{a^2}{\Sigma_{ii}} = [a \quad b] \begin{bmatrix} 1 + \frac{1}{\Sigma_{ii}} & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \quad (14)$$

$$= [a \quad b] \begin{bmatrix} \Sigma_{ii} & -\Sigma_{ii} \\ -\Sigma_{ii} & 1 + \Sigma_{ii} \end{bmatrix}^{-1} \begin{bmatrix} a \\ b \end{bmatrix}, \quad (15)$$

thus revealing the integrand of (13) to be (proportional to) a bivariate Gaussian PDF. The innermost integral of (13) is therefore equivalent to marginalizing out one of the variables in this bivariate distribution, up to a normalizing constant which can be pulled from the constants in front of the integral. Continuing the derivation in this way gives

$$\mathbb{E}[x_i] = \frac{1}{\sqrt{2\pi(1 + \Sigma_{ii})}} \int_{-\infty}^{\mu_i} \exp\left(-\frac{b^2}{2(1 + \Sigma_{ii})}\right) db \quad (16)$$

$$= \Phi(\mu_i, 0, 1 + \Sigma_{ii}) = \Phi\left(\frac{\mu_i}{\sqrt{1 + \Sigma_{ii}}}\right). \quad (17)$$

To derive the second raw moments associated with the probit transform, we begin with an approach similar to the one above. We start with the product moment $\mathbb{E}[x_i x_j]$ (for notational simplicity, let $\Sigma_{(i,j)} = \begin{bmatrix} \Sigma_{ii} & \Sigma_{ij} \\ \Sigma_{ji} & \Sigma_{jj} \end{bmatrix}$):

$$\mathbb{E}[x_i x_j] = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Phi(w_1) \Phi(w_2) \phi\left(\left[\begin{array}{c} w_1 \\ w_2 \end{array}\right], \left[\begin{array}{c} \mu_i \\ \mu_j \end{array}\right], \Sigma_{(i,j)}\right) dw_1 dw_2 \quad (18)$$

$$= \frac{1}{4\pi^2 |\Sigma_{(i,j)}|^{1/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{w_1} \int_{-\infty}^{w_2} \exp\left(-\frac{1}{2} \left(\left[\begin{array}{c} w_1 - \mu_i \\ w_2 - \mu_j \end{array}\right]^{\top} \Sigma_{(i,j)}^{-1} \left[\begin{array}{c} w_1 - \mu_i \\ w_2 - \mu_j \end{array}\right]\right)\right) \exp\left(-\frac{1}{2} (z_1^2 + z_2^2)\right) dz_2 dz_1 dw_2 dw_1. \quad (19)$$

Next, we make the following substitutions: $a_1 = w_1 - \mu_i$, $a_2 = w_2 - \mu_j$, $b_1 = z_1 - a_1$ and $b_2 = z_2 - a_2$:

$$\mathbb{E}[x_i x_j] = \frac{1}{4\pi^2 |\Sigma_{(i,j)}|^{1/2}} \int_{-\infty}^{\mu_i} \int_{-\infty}^{\mu_j} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2} \left(\left[\begin{array}{c} a_1 \\ a_2 \end{array}\right]^{\top} \Sigma_{(i,j)}^{-1} \left[\begin{array}{c} a_1 \\ a_2 \end{array}\right]\right)\right) \exp\left(-\frac{1}{2} ((a_1 + b_1)^2 + (a_2 + b_2)^2)\right) da_2 da_1 db_2 db_1. \quad (20)$$

We can again express the exponent in (20) using matrix notation as follows

$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}^{\top} \Sigma_{(i,j)}^{-1} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} + (a_1 + b_1)^2 + (a_2 + b_2)^2 = \begin{bmatrix} a_1 \\ a_2 \\ b_1 \\ b_2 \end{bmatrix}^{\top} \begin{bmatrix} \Sigma_{(i,j)}^{-1} & I_2 \\ I_2 & I_2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ b_1 \\ b_2 \end{bmatrix}, \quad (21)$$

where I_2 is the 2-by-2 identity matrix. In this form, we can recognize the integrand of (20) to be proportional to a multivariate Gaussian PDF. Pulling constants from outside the integral gives

$$\mathbb{E}[x_i x_j] = \int_{-\infty}^{\mu_i} \int_{-\infty}^{\mu_j} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi\left(\left[\begin{array}{c} a_1 \\ a_2 \\ b_1 \\ b_2 \end{array}\right], \left[\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \end{array}\right], \left[\begin{array}{cc} \Sigma_{(i,j)} & -\Sigma_{(i,j)} \\ -\Sigma_{(i,j)} & \Sigma_{(i,j)} + I_2 \end{array}\right]\right) da_2 da_1 db_2 db_1. \quad (22)$$

Thus, the two innermost integrals correspond to marginalizing out the variable a_1 and a_2 from this multivariate Gaussian and so we arrive at the final result:

$$\mathbb{E}[x_i x_j] = \int_{-\infty}^{\mu_i} \int_{-\infty}^{\mu_j} \phi\left(\left[\begin{array}{c} b_1 \\ b_2 \end{array}\right], \left[\begin{array}{c} 0 \\ 0 \end{array}\right], \Sigma_{(i,j)} + I_2\right) db_2 db_1 = \Phi\left(\left[\begin{array}{c} \mu_i \\ \mu_j \end{array}\right], \Sigma_{(i,j)} + I_2\right). \quad (23)$$

Using the same derivation as detailed above, we can show that

$$\mathbb{E}[x_i^2] = \Phi\left(\left[\begin{array}{c} \mu_i \\ \mu_i \end{array}\right], \left[\begin{array}{cc} \Sigma_{ii} + 1 & \Sigma_{ii} \\ \Sigma_{ii} & \Sigma_{ii} + 1 \end{array}\right]\right). \quad (24)$$

Again, we present the relevant partial derivatives, starting with the partial derivatives of the first moment:

$$\frac{\partial \mathbb{E}[x_i]}{\partial \mu_i} = \phi \left(\frac{\mu_i}{\sqrt{1 + \Sigma_{ii}}} \right) \frac{1}{\sqrt{1 + \Sigma_{ii}}} \quad (25)$$

$$\frac{\partial \mathbb{E}[x_i]}{\partial \Sigma_{ii}} = \phi \left(\frac{\mu_i}{\sqrt{1 + \Sigma_{ii}}} \right) \frac{-\mu_i}{2(1 + \Sigma_{ii})^{3/2}}, \quad (26)$$

which follow from the fundamental theorem of calculus and the chain rule. The derivative of the second raw moments w.r.t. μ_i can also be computed in a similar fashion:

$$\begin{aligned} \frac{\partial \mathbb{E}[x_i^2]}{\partial \mu_i} &= \frac{\partial}{\partial \mu_i} \Phi \left(\begin{bmatrix} \mu_i \\ \mu_i \end{bmatrix}, \begin{bmatrix} \Sigma_{ii} + 1 & \Sigma_{ii} \\ \Sigma_{ii} & \Sigma_{ii} + 1 \end{bmatrix} \right) \\ &= \int_{-\infty}^{\mu_i} \phi \left(\begin{bmatrix} b_1 \\ \mu_i \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) db_1 \\ &\quad + \int_{-\infty}^{\mu_i} \phi \left(\begin{bmatrix} \mu_i \\ b_2 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) db_2 \\ &= 2 \int_{-\infty}^{\mu_i} \phi \left(\begin{bmatrix} \mu_i \\ b \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) db \\ &= 2 \left(\phi \left(\frac{\mu_i}{\sqrt{1 + \Sigma_{ii}}} \right) \right. \\ &\quad \left. \Phi \left(\mu_i, \frac{\Sigma_{ii}}{\Sigma_{ii} + 1} \mu_i, \frac{\Sigma_{ii}}{\Sigma_{ii} + 1} + 1 \right) \right) \quad (27) \end{aligned}$$

where the last line can be arrived at by pulling the term $\phi(\mu_i/\sqrt{1+\Sigma_{ii}})$ out of the integral and then completing the square. Following a similar derivation, the partial derivative of the product moment w.r.t. μ_i is

$$\begin{aligned} \frac{\partial \mathbb{E}[x_i x_j]}{\partial \mu_i} &= \phi \left(\frac{\mu_i}{\sqrt{1 + \Sigma_{ii}}} \right) \\ &\quad \Phi \left(\mu_j, \frac{\Sigma_{ij}}{\Sigma_{ii} + 1} \mu_i, \Sigma_{jj} + 1 - \frac{\Sigma_{ij}^2}{\Sigma_{ii} + 1} \right). \quad (28) \end{aligned}$$

Next, the partial derivative of the second moment w.r.t. the covariance can be computed as follows:

$$\begin{aligned} \frac{\partial \mathbb{E}[x_i x_j]}{\partial \Sigma_{ij}} &= -\frac{\Sigma_{ij}}{|\Sigma_{(i,j)}|} \left(\Phi \left(\begin{bmatrix} \mu_i \\ \mu_j \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) \right. \\ &\quad + \int_{-\infty}^{\mu_i} \int_{-\infty}^{\mu_j} \phi \left(\begin{bmatrix} \mu_i \\ \mu_j \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) \\ &\quad \left. \left(\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}^\top \Sigma_{(i,j)}^{-1} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} - \frac{b_1 b_2}{\Sigma_{ij}} \right) db_2 db_1 \right). \quad (29) \end{aligned}$$

The second term can be decomposed into a weighted sum of the second raw moments of a truncated bivariate Gaussian. These moments can be expressed in terms

of the univariate Gaussian PDF and CDF [4]:

$$\begin{aligned} &\int_{-\infty}^{\mu_i} \int_{-\infty}^{\mu_j} b_1^2 \phi \left(\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) db_2 db_1 \\ &= (\Sigma_{ii} + 1) \left(\Phi \left(\begin{bmatrix} \mu_i \\ \mu_j \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) \right. \\ &\quad - t_1(\mu_i^*, \mu_j^*, \rho) - \rho^2 t_2(\mu_i^*, \mu_j^*, \rho) \\ &\quad \left. + \rho \sqrt{1 - \rho^2} t_3(\mu_i^*, \mu_j^*, \rho) \right) \quad (30) \end{aligned}$$

where

$$\rho = \frac{\Sigma_{ij}^2}{(\Sigma_{ii} + 1)(\Sigma_{jj} + 1)} \quad (31)$$

$$\mu_i^* = \frac{\mu_i}{\Sigma_{ii} + 1} \quad (32)$$

$$\mu_j^* = \frac{\mu_j}{\Sigma_{jj} + 1} \quad (33)$$

$$t_1(\mu_i^*, \mu_j^*, \rho) = \mu_i^* \phi(\mu_i^*) \Phi \left(\frac{\mu_j^* - \rho \mu_i^*}{\sqrt{1 - \rho^2}} \right) \quad (34)$$

$$t_2(\mu_i^*, \mu_j^*, \rho) = \mu_j^* \phi(\mu_j^*) \Phi \left(\frac{\mu_i^* - \rho \mu_j^*}{\sqrt{1 - \rho^2}} \right) \quad (35)$$

$$t_3(\mu_i^*, \mu_j^*, \rho) = \frac{1}{\sqrt{2\pi}} \phi \left(\sqrt{\frac{\mu_i^{*2} - 2\rho\mu_i^* \mu_j^* + \mu_j^{*2}}{1 - \rho^2}} \right). \quad (36)$$

Similarly, the other moments of the truncated bivariate Gaussian are

$$\begin{aligned} &\int_{-\infty}^{\mu_i} \int_{-\infty}^{\mu_j} b_2^2 \phi \left(\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) db_2 db_1 \\ &= (\Sigma_{jj} + 1) \left(\Phi \left(\begin{bmatrix} \mu_i \\ \mu_j \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) \right. \\ &\quad - \rho^2 t_1(\mu_i^*, \mu_j^*, \rho) - t_2(\mu_i^*, \mu_j^*, \rho) \\ &\quad \left. + \rho \sqrt{1 - \rho^2} t_3(\mu_i^*, \mu_j^*, \rho) \right) \quad (37) \end{aligned}$$

and

$$\begin{aligned} &\int_{-\infty}^{\mu_i} \int_{-\infty}^{\mu_j} b_1 b_2 \phi \left(\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) db_2 db_1 \\ &= \rho \sqrt{(\Sigma_{ii} + 1)(\Sigma_{jj} + 1)} \\ &\quad \left(\Phi \left(\begin{bmatrix} \mu_i \\ \mu_j \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) - t_1(\mu_i^*, \mu_j^*, \rho) \right. \\ &\quad \left. - t_2(\mu_i^*, \mu_j^*, \rho) + \frac{\sqrt{1 - \rho^2}}{\rho} t_3(\mu_i^*, \mu_j^*, \rho) \right). \quad (38) \end{aligned}$$

We can therefore substitute (30), (37) and (38) into (29) to come up with a closed form for this partial

derivative. Lastly, the partial derivatives of the second raw moments w.r.t. Σ_{ii} are

$$\begin{aligned} \frac{\partial \mathbb{E}[x_i x_j]}{\partial \Sigma_{ii}} &= -\frac{\Sigma_{jj} + 1}{2|\Sigma_{(i,j)}|} \left(\Phi \left(\begin{bmatrix} \mu_i \\ \mu_j \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) \right. \\ &\quad \left. + \int_{-\infty}^{\mu_i} \int_{-\infty}^{\mu_j} \phi \left(\begin{bmatrix} \mu_i \\ \mu_j \end{bmatrix}, \Sigma_{(i,j)} + I_2 \right) \right. \\ &\quad \left. \left(\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}^\top \Sigma_{(i,j)}^{-1} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} + \frac{b_2^2}{\Sigma_{jj} + 1} \right) db_2 db_1 \right) \end{aligned} \quad (39)$$

and

$$\begin{aligned} \frac{\partial \mathbb{E}[x_i^2]}{\partial \Sigma_{ii}} &= -\frac{1}{2\Sigma_{ii} + 1} \left(\Phi \left(\begin{bmatrix} \mu_i \\ \mu_i \end{bmatrix}, \begin{bmatrix} \Sigma_{ii} + 1 & \Sigma_{ii} \\ \Sigma_{ii} & 1 + \Sigma_{ii} \end{bmatrix} \right) \right. \\ &\quad \left. - \int_{-\infty}^{\mu_i} \int_{-\infty}^{\mu_i} \phi \left(\begin{bmatrix} \mu_i \\ \mu_i \end{bmatrix}, \begin{bmatrix} \Sigma_{ii} + 1 & \Sigma_{ii} \\ \Sigma_{ii} & 1 + \Sigma_{ii} \end{bmatrix} \right) \right. \\ &\quad \left. \left(\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}^\top \begin{bmatrix} \Sigma_{ii} & \Sigma_{ii} + 1 \\ \Sigma_{ii} + 1 & \Sigma_{ii} \end{bmatrix}^{-1} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \right) db_2 db_1 \right). \end{aligned} \quad (40)$$

We can again substitute (30), (37) and (38) into (39) and (40) to come up with closed forms for these partial derivatives.

References

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