

# Supplementary material for: Spike and Slab Variational Inference for Multi-Task and Multiple Kernel Learning

In this extra material, we provide more details about the variational EM algorithm for multi-task and multiple kernel learning (Section 1) as well as the updates for the paired Gibbs sampler (Section 2).

## 1 Variational EM algorithm for multi-task and multiple kernel learning

The joint probability density function is

$$\begin{aligned} p(\mathbf{Y}, \widetilde{\mathbf{W}}, \mathbf{S}, \Phi) &= \prod_{q=1}^Q \mathcal{N}(\mathbf{y}_q | \sum_{m=1}^M s_{qm} \widetilde{w}_{qm} \phi_m, \sigma_q^2) \\ &\times \prod_{q=1}^Q \prod_{m=1}^M [\mathcal{N}(\widetilde{w}_{qm} | 0, \sigma_w^2) \pi^{s_{qm}} (1 - \pi)^{1-s_{qm}}] \prod_{m=1}^M \mathcal{N}(\phi_m | \mathbf{0}, \mathbf{K}_m), \end{aligned}$$

where the GP latent vector  $\phi_m \in \mathbb{R}^N$  and where we assumed zero-mean GPs for simplicity. The logarithm of the marginal likelihood is

$$\log p(\mathbf{Y}) = \log \sum_{\mathbf{S}} \int_{\mathbf{W}, \Phi} p(\mathbf{Y}, \widetilde{\mathbf{W}}, \mathbf{S}, \Phi) d\mathbf{W} d\Phi.$$

The variational Bayesian method maximizes the following Jensen's lower bound on the above log marginal likelihood

$$\mathcal{F} = \sum_{\mathbf{S}} \int_{\mathbf{W}, \Phi} q(\widetilde{\mathbf{W}}, \mathbf{S}, \Phi) \log \frac{p(\mathbf{Y}, \widetilde{\mathbf{W}}, \mathbf{S}, \Phi)}{q(\widetilde{\mathbf{W}}, \mathbf{S}, \Phi)} d\mathbf{W} d\Phi,$$

where the variational distribution is assumed to factorize as follows

$$q(\widetilde{\mathbf{W}}, \mathbf{S}, \Phi) = \prod_{q=1}^Q \prod_{m=1}^M q(\widetilde{w}_{qm}, s_{qm}) \prod_{m=1}^M q(\phi_m).$$

In the next two sections we present a variational EM algorithm for the maximization of this lower bound. Section 1.1 describes the E-step updates and section 1.2 describes the M-step updates. The whole algorithm is a standard variational EM and all its updates are used by our implementation together with a specialized update presented in section 1.3. More precisely, as mentioned in the main paper separately updating the factor  $q(\phi_m)$  of the GP latent vector and the hyperparameters  $\theta_m$  of the covariance function of the same GP exhibits slow convergence. This is because of the strong dependence of the hyperparameters  $\theta_m$  on posterior  $q(\phi_m)$ . Notice that an analogous problem arises when applying MCMC to GP models [1]. Section 1.3 shows how this problem can be solved by performing a joint update of  $(q(\phi_m), \theta_m)$ . Note that for clarity reasons we have made the choice to firstly present the regular EM updates and then the specialized step in order to gain a better understanding about the whole issue.

### 1.1 E-Step

The update for the factor  $q(\widetilde{w}_{qm}, s_{qm})$  is such that  $q(\widetilde{w}_{qm}, s_{qm}) = q(\widetilde{w}_{qm} | s_{qm}) q(s_{qm})$  where

$$\gamma_{qm} = q(s_{qm} = 1) = \frac{1}{1 + e^{-u_{qm}}}$$

$$u_{qm} = \log \frac{\pi}{1 - \pi} + \frac{1}{2} \log \frac{\sigma_q^2}{\sigma_w^2} - \frac{1}{2} \log \left( \langle \phi_m^T \phi_m \rangle + \frac{\sigma_q^2}{\sigma_w^2} \right) + \frac{1}{2\sigma_q^2} \frac{\left( \mathbf{y}_q^T \langle \phi_m \rangle - \sum_{k \neq m} \langle s_{qk} w_{qk} \rangle \langle \phi_m^T \rangle \langle \phi_k \rangle \right)^2}{\left( \langle \phi_m^T \phi_m \rangle + \frac{\sigma_q^2}{\sigma_w^2} \right)}$$

$$q(\tilde{w}_{qm}|s_{qm}=0) = \mathcal{N}(\tilde{w}_{qm}|0, \sigma_w^2)$$

$$\begin{aligned} q(\tilde{w}_{qm}|s_{qm}=1) &= \mathcal{N}\left(\tilde{w}_{qm} \middle| \frac{\langle \phi_m^T \rangle \mathbf{y}_q - \sum_{k \neq m} \langle s_{qk} w_{qk} \rangle \langle \phi_m^T \rangle \langle \phi_k \rangle}{\langle \phi_m^T \phi_m \rangle + \frac{\sigma_q^2}{\sigma_w^2}}, \frac{\sigma_q^2}{\langle \phi_m^T \phi_m \rangle + \frac{\sigma_q^2}{\sigma_w^2}}\right) \\ &= \mathcal{N}(\tilde{w}_{qm} | \mu_{w_{qm}}, \sigma_{w_{qm}}^2) \end{aligned} \quad (1)$$

So overall an update of  $q(\tilde{w}_{qm}, s_{qm})$  reduces to an update of the variational parameters  $(\mu_{w_{qm}}, \sigma_{w_{qm}}^2, \gamma_{qm})$ . In summary,  $q(\tilde{w}_{qm}, s_{qm})$  could be written as

$$q(\tilde{w}_{qm}|s_{qm}) \times q(s_{qm}) = \mathcal{N}(\tilde{w}_{qm}|s_{qm} \mu_{w_{qm}}, s_{qm} \sigma_{w_{qm}}^2 + (1 - s_{qm}) \sigma_w^2) \times \gamma_{qm}^{s_{qm}} (1 - \gamma_{qm})^{1-s_{qm}}.$$

Finally, note that under the distribution  $q(\tilde{w}_{qm}, s_{qm})$ , the expectation  $\langle s_{qm} w_{qm} \rangle = \gamma_{qm} \mu_{w_{qm}}$ .

The variational update for each factor  $q(\phi_m)$  can be computed as

$$q(\phi_m) = \mathcal{N}(\phi_m | \boldsymbol{\mu}_{\phi_m}, \boldsymbol{\Sigma}_{\phi_m})$$

where

$$\boldsymbol{\Sigma}_{\phi_m} = \left( \sum_{q=1}^Q \frac{\langle s_{qm} \tilde{w}_{qm}^2 \rangle}{\sigma_q^2} \mathbf{I} + \mathbf{K}_m^{-1} \right)^{-1}$$

and

$$\boldsymbol{\mu}_{\phi_m} = \boldsymbol{\Sigma}_{\phi_m} \sum_{q=1}^Q \frac{\langle s_{qm} \tilde{w}_{qm} \rangle}{\sigma_q^2} \left( \mathbf{y}_q - \sum_{k \neq m} \langle s_{qk} \tilde{w}_{qk} \rangle \langle \phi_k \rangle \right)$$

where  $\langle s_{qm} \tilde{w}_{qm}^2 \rangle = \gamma_{qm} (\mu_{w_{qm}}^2 + \sigma_{w_{qm}}^2)$ . Also the expectation  $\langle \phi_m^T \phi_m \rangle = \boldsymbol{\mu}_{\phi_m}^T \boldsymbol{\mu}_{\phi_m} + \text{tr}(\boldsymbol{\Sigma}_{\phi_m})$ .

Notice that the update for  $\boldsymbol{\Sigma}_{\phi_m}$  depends on the inverse  $\mathbf{K}_m^{-1}$  which is not numerically stable as  $\mathbf{K}_m$  in computer precision might not be invertible. This, however, is easily resolved by re-writing  $\boldsymbol{\Sigma}_{\phi_m}$  as

$$\boldsymbol{\Sigma}_{\phi_m} = \mathbf{K}_m (\alpha_m \mathbf{K}_m + I)^{-1},$$

where  $\alpha_m = \sum_{q=1}^Q \frac{\langle s_{qm} \tilde{w}_{qm}^2 \rangle}{\sigma_q^2}$  is just a scalar. This now can be implemented in a symmetric and numerically stable way through the use of the Cholesky decomposition (and inverse Cholesky) of  $(\alpha_m \mathbf{K}_m + I)$ .

## 1.2 M-step

In the M-step, the bound is maximized w.r.t. hyperparameters  $\{\{\sigma_q^2\}_{q=1}^Q, \sigma_w^2, \pi\}$  and the kernel hyperparameters  $\boldsymbol{\Theta} = \{\boldsymbol{\theta}_m\}_{m=1}^M$ . The first set of hyperparameters is maximized using analytical updates. On the other hand, kernel hyperparameters require nonlinear gradient-based optimization.

The explicit form of the variational lower bound is

$$\begin{aligned}
\mathcal{F} = & -\frac{QN}{2} \log(2\pi) - \frac{N}{2} \sum_{q=1}^Q \log(\sigma_q^2) - \frac{1}{2} \sum_{q=1}^Q \frac{\mathbf{y}_q^T \mathbf{y}_q}{\sigma_q^2} & \% \mathcal{F}_1 \\
& + \sum_{m=1}^M \left( \sum_{q=1}^Q \frac{\langle s_{qm} \tilde{w}_{qm} \rangle}{\sigma_q^2} \mathbf{y}_q \right)^T \langle \phi_m \rangle & \% \mathcal{F}_2 \\
& - \frac{1}{2} \sum_{m=1}^M \left( \sum_{q=1}^Q \frac{\langle s_{qm} \tilde{w}_{qm}^2 \rangle}{\sigma_q^2} \right) \langle \phi_m \phi_m^T \rangle & \% \mathcal{F}_3 \\
& - \sum_{m=1}^M \left( \sum_{m'=m+1}^M \left( \sum_{q=1}^Q \frac{\langle s_{qm} \tilde{w}_{qm} \rangle \langle s_{qm'} \tilde{w}_{qm'} \rangle}{\sigma_q^2} \right) \langle \phi_{m'} \rangle \right)^T \langle \phi_m \rangle & \% \mathcal{F}_4 \\
& - \frac{MQ}{2} \log(2\pi\sigma_w^2) - \frac{1}{2\sigma_w^2} \sum_{q=1}^Q \sum_{m=1}^M \langle \tilde{w}_{qm}^2 \rangle & \% \mathcal{F}_5 \\
& + \log(\pi) \sum_{q=1}^Q \sum_{m=1}^M \langle s_{qm} \rangle + \log(1-\pi) \sum_{q=1}^Q \sum_{m=1}^M \langle 1-s_{qm} \rangle & \% \mathcal{F}_6 \\
& - \frac{MN}{2} \log(2\pi) - \frac{1}{2} \sum_{m=1}^M (\log |\mathbf{K}_m| + \text{tr}[\mathbf{K}_m^{-1} \langle \phi_m \phi_m^T \rangle]) & \% \mathcal{F}_7 \\
& + \frac{MQ}{2} \log(2e\pi\sigma_w^2) - \frac{1}{2} \log \sigma_w^2 \sum_{q=1}^Q \sum_{m=1}^M \langle s_{qm} \rangle + \frac{1}{2} \sum_{q=1}^Q \sum_{m=1}^M \langle s_{qm} \rangle \log \sigma_{w_{qm}}^2 & \% \mathcal{E}_1 \\
& - \sum_{q=1}^Q \sum_{m=1}^M [\langle 1-s_{qm} \rangle \log \langle 1-s_{qm} \rangle - \langle s_{qm} \rangle \log \langle s_{qm} \rangle] & \% \mathcal{E}_2 \\
& + \frac{MN}{2} \log(2\pi) + \frac{MN}{2} + \frac{1}{2} \sum_{m=1}^M \log |\Sigma_{\phi_m}| & \% \mathcal{E}_3
\end{aligned} \tag{2}$$

The  $\mathcal{F}_5$  term can be further simplified by using the fact that  $\langle \tilde{w}_{qm}^2 \rangle = \gamma_{qm}(\mu_{w_{qm}}^2 + \sigma_{w_{qm}}^2) + (1 - \gamma_{qm})\sigma_w^2$ . Also some terms above cancel out such as the term  $\frac{MQ}{2} \log(2\pi\sigma_w^2)$ .

Finally, the updates for the hyperparameters are as follows

$$\begin{aligned}
\sigma_q^2 &= \frac{1}{N} \text{tr}[\mathbf{y}_q \mathbf{y}_q^T - \mathbf{y}_q \sum_{m=1}^M \langle s_{qm} \tilde{w}_{qm} \rangle \langle \phi_m \rangle^T + \sum_{m=1}^M \langle s_{qm} \tilde{w}_{qm}^2 \rangle \langle \phi_m \phi_m^T \rangle + 2 \sum_{m>m'} \langle s_{qm} \tilde{w}_{qm} \rangle \langle s_{qm'} \tilde{w}_{qm'} \rangle \langle \phi_m \rangle \langle \phi_{m'} \rangle] \\
\sigma_w^2 &= \frac{\sum_{q=1}^Q \sum_{m=1}^M \gamma_{qm}(\mu_{w_{qm}}^2 + \sigma_{w_{qm}}^2)}{\sum_{q=1}^Q \sum_{m=1}^M \gamma_{qm}} \\
\pi &= \frac{1}{MQ} \sum_{q=1}^Q \sum_{m=1}^M \langle s_{qm} \rangle \\
\boldsymbol{\theta}_m &= \arg \max_{\boldsymbol{\theta}_m} \left[ -\frac{1}{2} \log |\mathbf{K}_m| - \frac{1}{2} \text{tr}[\mathbf{K}_m^{-1} \langle \phi_m \phi_m^T \rangle] \right]
\end{aligned}$$

where anything in brackets  $\langle \cdot \rangle$  is computed under the current value of the variational distribution and is assumed to be fixed (given from the E-step).

### 1.3 A joint update for $q(\phi_m)$ and $\boldsymbol{\theta}_m$

Notice that the update for the hyperparameter  $\boldsymbol{\theta}_m$ , which parameterize  $\mathbf{K}_m$ , is problematic for two reasons. Firstly, it requires the inverse of  $\mathbf{K}_m$  and this is numerically unstable as

in (computer precision) such an inverse might not exist. Of course, such a problem can be partially overcome by adding a small amount of “jitter” into the diagonal of  $\mathbf{K}_m$ , which however is not ideal. Secondly, the update of the hyperparameters  $\boldsymbol{\theta}_m$  strongly depends on the statistic  $\langle \phi_m \phi_m^T \rangle$  computed under the factor  $q(\phi_m)$  which is fixed. The update of  $\boldsymbol{\theta}_m$  can be “slow” because  $\langle \phi_m \phi_m^T \rangle$  depends on the kernel matrix  $\mathbf{K}_m^{old}$  evaluated at the old values of the hyperparameter  $\boldsymbol{\theta}_m^{old}$ . To resolve this, we would like to update simultaneously somehow  $\boldsymbol{\theta}_m$  and the statistic  $\langle \phi_m \phi_m^T \rangle$ , i.e. the factor  $q(\phi_m)$ . This can be done in an elegant and efficient way using a Marginalized Variational step [2]. Next we describe the whole idea.

We would like to perform a joint optimization update for  $(q(\phi_m), \boldsymbol{\theta}_m)$  in a way that the factor  $q(\phi_m)$  is marginalized/removed optimally from the optimization problem. We write the variational lower bound as follows

$$\mathcal{F}(\boldsymbol{\theta}_m) = \int q(\phi_m) q(\Theta) \log \frac{p(\mathbf{Y}, \phi_m, \Theta) p(\Theta) \mathcal{N}(\phi_m | \mathbf{0}, \mathbf{K}_m)}{q(\phi_m) q(\Theta)} d\phi_m d\Theta,$$

where  $\Theta$  are all random variables excluding  $\phi_m$  and  $q(\Theta)$  their variational distribution. Given that we wish to update the factor  $q(\phi_m)$  and the kernel matrix  $\mathbf{K}_m$  while the rest are just constants, the above is written as

$$\mathcal{F}(\boldsymbol{\theta}_m) = \int q(\phi_m) q(\Theta) \log \frac{p(\mathbf{Y}, \phi_m, \Theta) \mathcal{N}(\phi_m | \mathbf{0}, \mathbf{K}_m)}{q(\phi_m)} d\phi_m d\Theta + const.$$

Now the optimal  $q(\phi_m)$  is

$$q(\phi_m) = \frac{\exp(\langle \log p(\mathbf{Y}, \phi_m, \Theta) \rangle_{q(\Theta)}) \mathcal{N}(\phi_m | \mathbf{0}, \mathbf{K}_m)}{\int \exp(\langle \log p(\mathbf{Y}, \phi_m, \Theta) \rangle_{q(\Theta)}) \mathcal{N}(\phi_m | \mathbf{0}, \mathbf{K}_m) d\phi_m}$$

Substituting this optimal  $q(\phi_m)$  back into the bound we obtain

$$\mathcal{F}(\boldsymbol{\theta}_m) = \log \int \exp(\langle \log p(\mathbf{Y}, \phi_m, \Theta) \rangle_{q(\Theta)}) \mathcal{N}(\phi_m | \mathbf{0}, \mathbf{K}_m) d\phi_m + const.$$

This now is analytically tractable and can neatly be written as the marginal likelihood of a standard GP regression model:

$$\mathcal{F}(\boldsymbol{\theta}_m) = \log \mathcal{N}(\bar{\mathbf{y}} | \mathbf{0}, \mathbf{K}_m + \alpha_m^{-1} I) + const$$

where

$$\bar{\mathbf{y}} = \frac{1}{\alpha_m} \sum_{q=1}^Q \frac{\langle s_{qm} \tilde{w}_{qm} \rangle}{\sigma_q^2} \left( \mathbf{y}_q - \sum_{k \neq m} \langle s_{qk} \tilde{w}_{qk} \rangle \langle \phi_k \rangle \right)$$

are like fixed pseudo-data and

$$\alpha_m = \sum_{q=1}^Q \frac{\langle s_{qm} \tilde{w}_{qm}^2 \rangle}{\sigma_q^2}$$

is a fixed inverse noise variance parameter. The above now is optimized wrt  $\boldsymbol{\theta}_m$  and this can be done by using any standard GP implementation for maximizing the marginal likelihood of a GP standard regression model (we will only need to keep fixed the noise variance  $\alpha_m^{-1}$ ). Notice that the optimization requires the inverse of  $\mathbf{K}_m + \alpha_m^{-1} I$  which often will be numerically stable due to the addition of  $\alpha_m^{-1}$  in the diagonal of  $\mathbf{K}_m$ .

Once the optimization is completed, we evaluate the final value of the factor  $q(\phi_m)$  and then continue with other variational EM updates.

## 2 Paired Gibbs sampling for spike and slab linear regression

Consider a single-output regression model:

$$p(\mathbf{y}, \tilde{\mathbf{w}}, \mathbf{s}) = \mathcal{N}(\mathbf{y} | \sum_{m=1}^M s_m \tilde{w}_m \mathbf{x}_m, \sigma^2 \mathbf{I}) \prod_{m=1}^M [\mathcal{N}(\tilde{w}_m | 0, \sigma_w^2) [\pi^{s_m} (1 - \pi)^{1-s_m}]]$$

The paired Gibbs sampler iteratively samples from the following conditional

$$p(\tilde{w}_m, s_m | \tilde{w}_{\setminus m}, s_{\setminus m}, \mathbf{y}) = p(\tilde{w}_m | s_m, \tilde{w}_{\setminus m}, s_{\setminus m}, \mathbf{y}) p(s_m | \tilde{w}_{\setminus m}, s_{\setminus m}, \mathbf{y}).$$

$p(s_m = 1 | \tilde{w}_{\setminus m}, s_{\setminus m}, \mathbf{y})$  is obtained analytically to be

$$\begin{aligned} p(s_m = 1 | \tilde{w}_{\setminus m}, s_{\setminus m}, \mathbf{y}) &= \frac{\pi \mathcal{N}(\mathbf{y} | \sum_{k \neq m} s_k \tilde{w}_k \mathbf{x}_k, \sigma^2 \mathbf{I} + \sigma_w^2 \mathbf{x}_m \mathbf{x}_m^T)}{\pi \mathcal{N}(\mathbf{y} | \sum_{k \neq m} s_k \tilde{w}_k \mathbf{x}_k, \sigma^2 \mathbf{I} + \sigma_w^2 \mathbf{x}_m \mathbf{x}_m^T) + (1 - \pi) \mathcal{N}(\mathbf{y} | \sum_{k \neq m} s_k \tilde{w}_k \mathbf{x}_k, \sigma^2 \mathbf{I})} \\ &= \frac{\pi \mathcal{N}(\mathbf{y} | \mathbf{b}_m, \sigma^2 \mathbf{I} + \sigma_w^2 \mathbf{x}_m \mathbf{x}_m^T)}{\pi \mathcal{N}(\mathbf{y} | \mathbf{b}_m, \sigma^2 \mathbf{I} + \sigma_w^2 \mathbf{x}_m \mathbf{x}_m^T) + (1 - \pi) \mathcal{N}(\mathbf{y} | \mathbf{b}_m, \sigma^2 \mathbf{I})} \end{aligned}$$

where

$$\mathbf{b}_m = \sum_{k \neq m} s_k \tilde{w}_k \mathbf{x}_k$$

A computationally more efficient expression can be obtained by applying matrix inversion lemma:

$$p(s_m = 1 | \tilde{w}_{\setminus m}, s_{\setminus m}, \mathbf{y}) = \sigma(u_m)$$

where  $\sigma(u_m) = \frac{1}{1 + e^{-u_m}}$  and

$$\begin{aligned} u_m &= \log \frac{\pi}{1 - \pi} + \frac{1}{2} \log \frac{\sigma^2}{\sigma_w^2} - \frac{1}{2} \log \left( \mathbf{x}_m^T \mathbf{x}_m + \frac{\sigma^2}{\sigma_w^2} \right) + \frac{1}{2\sigma^2} \frac{\left( \mathbf{x}_m^T \mathbf{y} - \sum_{k \neq m} s_k \tilde{w}_k \mathbf{x}_m^T \mathbf{x}_k \right)^2}{\left( \mathbf{x}_m^T \mathbf{x}_m + \frac{\sigma^2}{\sigma_w^2} \right)} \\ &= \log \frac{\pi}{1 - \pi} + \frac{1}{2} \log \frac{\sigma^2}{\sigma_w^2} - \frac{1}{2} \log \left( \mathbf{x}_m^T \mathbf{x}_m + \frac{\sigma^2}{\sigma_w^2} \right) + \frac{1}{2\sigma^2} \frac{(\mathbf{x}_m^T \mathbf{y} - \mathbf{x}_m^T \mathbf{b}_m)^2}{\left( \mathbf{x}_m^T \mathbf{x}_m + \frac{\sigma^2}{\sigma_w^2} \right)} \end{aligned}$$

Also,  $p(\tilde{w}_m | s_m = 0, \tilde{w}_{\setminus m}, s_{\setminus m}, \mathbf{y}) = \mathcal{N}(\tilde{w}_m | 0, \sigma_w^2)$  and  $p(\tilde{w}_m | s_m = 1, \tilde{w}_{\setminus m}, s_{\setminus m}, \mathbf{y})$  is

$$p(\tilde{w}_m | s_m = 1, \tilde{w}_{\setminus m}, s_{\setminus m}, \mathbf{y}) = \mathcal{N} \left( \tilde{w}_m \left| \frac{\mathbf{x}_m^T \mathbf{y} - \sum_{k \neq m} s_k \tilde{w}_k \mathbf{x}_m^T \mathbf{x}_k}{\mathbf{x}_m^T \mathbf{x}_m + \frac{\sigma^2}{\sigma_w^2}}, \frac{\sigma^2}{\mathbf{x}_m^T \mathbf{x}_m + \frac{\sigma^2}{\sigma_w^2}} \right. \right)$$

## References

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