

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

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

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 θ_m of the covariance function of the same GP exhibits slow convergence. This is because of the strong dependence of the hyperparameters θ_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

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

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

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

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

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

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

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 $\langle \boldsymbol{\phi}_m \boldsymbol{\phi}_m^T \rangle$ computed under the factor $q(\boldsymbol{\phi}_m)$ which is fixed. The update of $\boldsymbol{\theta}_m$ can be “slow” because $\langle \boldsymbol{\phi}_m \boldsymbol{\phi}_m^T \rangle$ 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 $\langle \boldsymbol{\phi}_m \boldsymbol{\phi}_m^T \rangle$, i.e. the factor $q(\boldsymbol{\phi}_m)$. 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 $(q(\boldsymbol{\phi}_m), \boldsymbol{\theta}_m)$ in a way that the factor $q(\boldsymbol{\phi}_m)$ is marginalized/removed optimally from the optimization problem. We write the variational lower bound as follows

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

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

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

Now the optimal $q(\boldsymbol{\phi}_m)$ is

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

Substituting this optimal $q(\boldsymbol{\phi}_m)$ back into the bound we obtain

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

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

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

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 α_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 α_m^{-1} in the diagonal of \mathbf{K}_m .

Once the optimization is completed, we evaluate the final value of the factor $q(\boldsymbol{\phi}_m)$ 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

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

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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