## 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

$$
\begin{aligned}
p(\mathbf{Y}, \widetilde{\mathbf{W}}, \mathbf{S}, \mathbf{\Phi}) & =\prod_{q=1}^{Q} \mathcal{N}\left(\mathbf{y}_{q} \mid \sum_{m=1}^{M} s_{q m} \widetilde{w}_{q m} \boldsymbol{\phi}_{m}, \sigma_{q}^{2}\right) \\
& \times \prod_{q=1}^{Q} \prod_{m=1}^{M}\left[\mathcal{N}\left(\widetilde{w}_{q m} \mid 0, \sigma_{w}^{2}\right) \pi^{s_{q m}}(1-\pi)^{s_{q m}}\right] \prod_{m=1}^{M} \mathcal{N}\left(\boldsymbol{\phi}_{m} \mid \mathbf{0}, \mathbf{K}_{m}\right)
\end{aligned}
$$

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

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

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

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

where the variational distribution is assumed to factorize as follows

$$
q(\widetilde{\mathbf{W}}, \mathbf{S}, \boldsymbol{\Phi})=\prod_{q=1}^{Q} \prod_{m=1}^{M} q\left(\widetilde{w}_{q m}, s_{q m}\right) \prod_{m=1}^{M} q\left(\boldsymbol{\phi}_{m}\right)
$$

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 $q\left(\boldsymbol{\phi}_{m}\right)$ of the GP latent vector and the hyperparameters $\boldsymbol{\theta}_{m}$ of the covariance function of the same GP exhibits slow convergence. This is because of the strong dependence of the hyperparameters $\boldsymbol{\theta}_{m}$ on posterior $q\left(\boldsymbol{\phi}_{m}\right)$. 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 $\left(q\left(\boldsymbol{\phi}_{m}\right), \boldsymbol{\theta}_{m}\right)$. 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 $q\left(\widetilde{w}_{q m}, s_{q m}\right)$ is such that $q\left(\widetilde{w}_{q m}, s_{q m}\right)=q\left(\widetilde{w}_{q m} \mid s_{q m}\right) q\left(s_{q m}\right)$ where

$$
\begin{gathered}
\gamma_{q m}=q\left(s_{q m}=1\right)=\frac{1}{1+e^{-u_{q m}}} \\
u_{q m}=\log \frac{\pi}{1-\pi}+\frac{1}{2} \log \frac{\sigma_{q}^{2}}{\sigma_{w}^{2}}-\frac{1}{2} \log \left(\left\langle\boldsymbol{\phi}_{m}^{\mathrm{T}} \boldsymbol{\phi}_{m}\right\rangle+\frac{\sigma_{q}^{2}}{\sigma_{w}^{2}}\right)+\frac{1}{2 \sigma_{q}^{2}} \frac{\left(\mathbf{y}_{q}^{\mathrm{T}}\left\langle\boldsymbol{\phi}_{m}\right\rangle-\sum_{k \neq m}\left\langle s_{q k} w_{q k}\right\rangle\left\langle\boldsymbol{\phi}_{m}^{\mathrm{T}}\right\rangle\left\langle\boldsymbol{\phi}_{k}\right\rangle\right)^{2}}{\left(\left\langle\boldsymbol{\phi}_{m}^{\mathrm{T}} \boldsymbol{\phi}_{m}\right\rangle+\frac{\sigma_{q}^{2}}{\sigma_{w}^{2}}\right)}
\end{gathered}
$$

$$
\begin{gather*}
q\left(\widetilde{w}_{q m} \mid s_{q m}=0\right)=\mathcal{N}\left(\widetilde{w}_{q m} \mid 0, \sigma_{w}^{2}\right) \\
q\left(\widetilde{w}_{q m} \mid s_{q m}=1\right)=\mathcal{N}\left(\widetilde{w}_{q m} \left\lvert\, \frac{\left\langle\boldsymbol{\phi}_{m}^{\mathrm{T}}\right\rangle \mathbf{y}_{q}-\sum_{k \neq m}\left\langle s_{q k} w_{q k}\right\rangle\left\langle\boldsymbol{\phi}_{m}^{\mathrm{T}}\right\rangle\left\langle\boldsymbol{\phi}_{k}\right\rangle}{\left\langle\boldsymbol{\phi}_{m}^{\mathrm{T}} \boldsymbol{\phi}_{m}\right\rangle+\frac{\sigma_{q}^{2}}{\sigma_{w}^{2}}}\right., \frac{\sigma_{q}^{2}}{\left\langle\boldsymbol{\phi}_{m}^{\mathrm{T}} \boldsymbol{\phi}_{m}\right\rangle+\frac{\sigma_{q}^{2}}{\sigma_{w}^{2}}}\right) \\
=\mathcal{N}\left(\widetilde{w}_{q m} \mid \mu_{w_{q m}}, \sigma_{w_{q m}}^{2}\right) \tag{1}
\end{gather*}
$$

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

$$
q\left(\widetilde{w}_{q m} \mid s_{q m}\right) \times q\left(s_{q m}\right)=\mathcal{N}\left(\widetilde{w}_{q m} \mid s_{q m} \mu_{w_{q m}}, s_{q m} \sigma_{w_{q m}}^{2}+\left(1-s_{q m}\right) \sigma_{w}^{2}\right) \times \gamma_{q m}^{s_{q m}}\left(1-\gamma_{q m}\right)^{1-s_{q m}}
$$

Finally, note that under the distribution $q\left(\widetilde{w}_{q m}, s_{q m}\right)$, the expectation $\left\langle s_{q m} w_{q m}\right\rangle=\gamma_{q m} \mu_{w_{q m}}$.
The variational update for each factor $q\left(\boldsymbol{\phi}_{m}\right)$ can be computed as

$$
q\left(\boldsymbol{\phi}_{m}\right)=\mathcal{N}\left(\boldsymbol{\phi}_{m} \mid \boldsymbol{\mu}_{\phi_{m}}, \boldsymbol{\Sigma}_{\phi_{m}}\right)
$$

where

$$
\boldsymbol{\Sigma}_{\phi_{m}}=\left(\sum_{q=1}^{Q} \frac{\left\langle s_{q m} \widetilde{w}_{q m}^{2}\right\rangle}{\sigma_{q}^{2}} \mathbf{I}+\mathbf{K}_{m}^{-1}\right)^{-1}
$$

and

$$
\boldsymbol{\mu}_{\phi_{m}}=\boldsymbol{\Sigma}_{\phi_{m}} \sum_{q=1}^{Q} \frac{\left\langle s_{q m} \widetilde{w}_{q m}\right\rangle}{\sigma_{q}^{2}}\left(\mathbf{y}_{q}-\sum_{k \neq m}\left\langle s_{q k} \widetilde{w}_{q k}\right\rangle\left\langle\boldsymbol{\phi}_{k}\right\rangle\right)
$$

where $\left\langle s_{q m} \widetilde{w}_{q m}^{2}\right\rangle=\gamma_{q m}\left(\mu_{w_{q m}}^{2}+\sigma_{w_{q m}}^{2}\right)$. Also the expectation $\left\langle\boldsymbol{\phi}_{m}^{\mathrm{T}} \boldsymbol{\phi}_{m}\right\rangle=\boldsymbol{\mu}_{\phi_{m}}^{\mathrm{T}} \boldsymbol{\mu}_{\phi_{m}}+\operatorname{tr}\left(\boldsymbol{\Sigma}_{\phi_{m}}\right)$.
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

$$
\Sigma_{\phi_{m}}=\mathbf{K}_{m}\left(\alpha_{m} \mathbf{K}_{m}+I\right)^{-1}
$$

where $\alpha_{m}=\sum_{q=1}^{Q} \frac{\left\langle s_{q m} \widetilde{w}_{q m}^{2}\right\rangle}{\sigma_{q}^{2}}$ 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 $\left(\alpha_{m} \mathbf{K}_{m}+I\right)$.

### 1.2 M-step

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

The explicit form of the variational lower bound is

$$
\begin{align*}
& \mathcal{F}=-\frac{Q N}{2} \log (2 \pi)-\frac{N}{2} \sum_{q=1}^{Q} \log \left(\sigma_{q}^{2}\right)-\frac{1}{2} \sum_{q=1}^{Q} \frac{\mathbf{y}_{q}^{\mathrm{T}} \mathbf{y}_{q}}{\sigma_{q}^{2}} \quad \quad \% \mathcal{F}_{\mathbf{1}} \\
& +\sum_{m=1}^{M}\left(\sum_{q=1}^{Q} \frac{\left\langle s_{q m} \widetilde{w}_{q m}\right\rangle}{\sigma_{q}^{2}} \mathbf{y}_{q}\right)^{\mathrm{T}}\left\langle\boldsymbol{\phi}_{m}\right\rangle \quad \% \mathcal{F}_{\mathbf{2}} \\
& -\frac{1}{2} \sum_{m=1}^{M}\left(\sum_{q=1}^{Q} \frac{\left\langle s_{q m} \widetilde{w}_{q m}^{2}\right\rangle}{\sigma_{q}^{2}}\right)\left\langle\boldsymbol{\phi}_{m} \boldsymbol{\phi}_{m}^{\mathrm{T}}\right\rangle \quad \% \mathcal{F}_{\mathbf{3}} \\
& -\sum_{m=1}^{M}\left(\sum_{m^{\prime}=m+1}^{M}\left(\sum_{q=1}^{Q} \frac{\left\langle s_{q m} \widetilde{w}_{q m}\right\rangle\left\langle s_{q m^{\prime}} \widetilde{w}_{q m^{\prime}}\right\rangle}{\sigma_{q}^{2}}\right)\left\langle\boldsymbol{\phi}_{m^{\prime}}\right\rangle\right)^{\mathrm{T}}\left\langle\boldsymbol{\phi}_{m}\right\rangle \quad \% \mathcal{F}_{\mathbf{4}} \\
& -\frac{M Q}{2} \log \left(2 \pi \sigma_{w}^{2}\right)-\frac{1}{2 \sigma_{w}^{2}} \sum_{q=1}^{Q} \sum_{m=1}^{M}\left\langle\widetilde{w}_{q m}^{2}\right\rangle \quad \% \mathcal{F}_{\mathbf{5}} \\
& +\log (\pi) \sum_{q=1}^{Q} \sum_{m=1}^{M}\left\langle s_{q m}\right\rangle+\log (1-\pi) \sum_{q=1}^{Q} \sum_{m=1}^{M}\left\langle 1-s_{q m}\right\rangle \quad \% \mathcal{F}_{6} \\
& -\frac{M N}{2} \log (2 \pi)-\frac{1}{2} \sum_{m=1}^{M}\left(\log \left|\mathbf{K}_{m}\right|+\operatorname{tr}\left[\mathbf{K}_{m}^{-1}\left\langle\boldsymbol{\phi}_{m} \boldsymbol{\phi}_{m}^{\mathrm{T}}\right\rangle\right]\right) \quad \quad \% \mathcal{F}_{\mathbf{7}} \\
& +\frac{M Q}{2} \log \left(2 e \pi \sigma_{w}^{2}\right)-\frac{1}{2} \log \sigma_{w}^{2} \sum_{q=1}^{Q} \sum_{m=1}^{M}\left\langle s_{q m}\right\rangle+\frac{1}{2} \sum_{q=1}^{Q} \sum_{m=1}^{M}\left\langle s_{q m}\right\rangle \log \sigma_{w_{q m}}^{2} \quad \% \mathcal{E}_{\mathbf{1}} \\
& -\sum_{q=1}^{Q} \sum_{m=1}^{M}\left[\left\langle 1-s_{q m}\right\rangle \log \left\langle 1-s_{q m}\right\rangle-\left\langle s_{q m}\right\rangle \log \left\langle s_{q m}\right\rangle\right] \quad \% \mathcal{E}_{\mathbf{2}} \\
& +\frac{M N}{2} \log (2 \pi)+\frac{M N}{2}+\frac{1}{2} \sum_{m=1}^{M} \log \left|\boldsymbol{\Sigma}_{\phi_{m}}\right| \quad \% \mathcal{E}_{\mathbf{3}} \tag{2}
\end{align*}
$$

The $\mathcal{F}_{5}$ term can be further simplified by using the fact that $\left\langle\widetilde{w}_{q m}^{2}\right\rangle=\gamma_{q m}\left(\mu_{w_{q m}}^{2}+\sigma_{w_{q m}}^{2}\right)+$ $\left(1-\gamma_{q m}\right) \sigma_{w}^{2}$. Also some terms above cancel out such as the term $\frac{M Q}{2} \log \left(2 \pi \sigma_{w}^{2}\right)$.

Finally, the updates for the hyperparameters are as follows

$$
\begin{gathered}
\sigma_{q}^{2}=\frac{1}{N} \operatorname{tr}\left[\mathbf{y}_{q} \mathbf{y}_{q}^{\mathrm{T}}-\mathbf{y}_{q} \sum_{m=1}^{M}\left\langle s_{q m} \widetilde{w}_{q m}\right\rangle\left\langle\boldsymbol{\phi}_{m}\right\rangle^{\mathrm{T}}+\sum_{m=1}^{M}\left\langle s_{q m} \widetilde{w}_{q m}^{2}\right\rangle\left\langle\boldsymbol{\phi}_{m} \boldsymbol{\phi}_{m}^{\mathrm{T}}\right\rangle+2 \sum_{m>m^{\prime}}\left\langle s_{q m} \widetilde{w}_{q m}\right\rangle\left\langle s_{q m^{\prime}} \widetilde{w}_{q m^{\prime}}\right\rangle\left\langle\boldsymbol{\phi}_{m}\right\rangle\left\langle\boldsymbol{\phi}_{m^{\prime}}\right\rangle\right] \\
\sigma_{w}^{2}=\frac{\sum_{q=1}^{Q} \sum_{m=1}^{M} \gamma_{q m}\left(\mu_{w_{q m}}^{2}+\sigma_{w_{q m}}^{2}\right)}{\sum_{q=1}^{Q} \sum_{m=1}^{M} \gamma_{q m}} \\
\pi=\frac{1}{M Q} \sum_{q=1}^{Q} \sum_{m=1}^{M}\left\langle s_{q m}\right\rangle \\
\boldsymbol{\theta}_{m}=\arg \max _{\boldsymbol{\theta}_{m}}\left[-\frac{1}{2} \log \left|\mathbf{K}_{m}\right|-\frac{1}{2} \operatorname{tr}\left[\mathbf{K}_{m}^{-1}\left\langle\boldsymbol{\phi}_{m} \boldsymbol{\phi}_{m}^{\mathrm{T}}\right\rangle\right]\right]
\end{gathered}
$$

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 $q\left(\boldsymbol{\phi}_{m}\right)$ 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 $\left\langle\boldsymbol{\phi}_{m} \boldsymbol{\phi}_{m}^{\mathrm{T}}\right\rangle$ computed under the factor $q\left(\boldsymbol{\phi}_{m}\right)$ which is fixed. The update of $\boldsymbol{\theta}_{m}$ can be "slow" because $\left\langle\boldsymbol{\phi}_{m} \boldsymbol{\phi}_{m}^{\mathrm{T}}\right\rangle$ depends on the kernel matrix $\mathbf{K}_{m}^{\text {old }}$ evaluated at the old values of the hyperparameter $\boldsymbol{\theta}_{m}^{\text {old }}$. To resolve this, we would like to update simultaneously somehow $\boldsymbol{\theta}_{m}$ and the statistic $\left\langle\boldsymbol{\phi}_{m} \boldsymbol{\phi}_{m}^{\mathrm{T}}\right\rangle$, i.e. the factor $q\left(\boldsymbol{\phi}_{m}\right)$. 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 $\left(q\left(\boldsymbol{\phi}_{m}\right), \boldsymbol{\theta}_{m}\right)$ in a way that the factor $q\left(\phi_{m}\right)$ is marginalized/removed optimally from the optimization problem. We write the variational lower bound as follows

$$
\mathcal{F}\left(\boldsymbol{\theta}_{m}\right)=\int q\left(\boldsymbol{\phi}_{m}\right) q(\Theta) \log \frac{p\left(\mathbf{Y}, \boldsymbol{\phi}_{m}, \Theta\right) p(\Theta) \mathcal{N}\left(\boldsymbol{\phi}_{m} \mid \mathbf{0}, \mathbf{K}_{m}\right)}{q\left(\boldsymbol{\phi}_{m}\right) q(\Theta)} d \boldsymbol{\phi}_{m} d \Theta
$$

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

$$
\mathcal{F}\left(\boldsymbol{\theta}_{m}\right)=\int q\left(\boldsymbol{\phi}_{m}\right) q(\Theta) \log \frac{p\left(\mathbf{Y}, \boldsymbol{\phi}_{m}, \Theta\right) \mathcal{N}\left(\boldsymbol{\phi}_{m} \mid \mathbf{0}, \mathbf{K}_{m}\right)}{q\left(\boldsymbol{\phi}_{m}\right)} d \boldsymbol{\phi}_{m} d \Theta+\text { const. }
$$

Now the optimal $q\left(\phi_{m}\right)$ is

$$
q\left(\boldsymbol{\phi}_{m}\right)=\frac{\exp ^{\left\langle\log p\left(\mathbf{Y}, \boldsymbol{\phi}_{m}, \Theta\right)\right\rangle_{q(\Theta)}} \mathcal{N}\left(\boldsymbol{\phi}_{m} \mid \mathbf{0}, \mathbf{K}_{m}\right)}{\int \exp ^{\left\langle\log p\left(\mathbf{Y}, \boldsymbol{\phi}_{m}, \Theta\right)\right\rangle_{q(\Theta)}} \mathcal{N}\left(\boldsymbol{\phi}_{m} \mid \mathbf{0}, \mathbf{K}_{m}\right) d \boldsymbol{\phi}_{m}}
$$

Substituting this optimal $q\left(\boldsymbol{\phi}_{m}\right)$ back into the bound we obtain

$$
\mathcal{F}\left(\boldsymbol{\theta}_{m}\right)=\log \int \exp ^{\left\langle\log p\left(\mathbf{Y}, \boldsymbol{\phi}_{m}, \Theta\right)\right\rangle_{q(\Theta)}} \mathcal{N}\left(\boldsymbol{\phi}_{m} \mid \mathbf{0}, \mathbf{K}_{m}\right) d \boldsymbol{\phi}_{m}+\text { const } .
$$

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

$$
\mathcal{F}\left(\boldsymbol{\theta}_{m}\right)=\log \mathcal{N}\left(\overline{\mathbf{y}} \mid \mathbf{0}, \mathbf{K}_{m}+\alpha_{m}^{-1} I\right)+\mathrm{const}
$$

where

$$
\overline{\mathbf{y}}=\frac{1}{\alpha_{m}} \sum_{q=1}^{Q} \frac{\left\langle s_{q m} \widetilde{w}_{q m}\right\rangle}{\sigma_{q}^{2}}\left(\mathbf{y}_{q}-\sum_{k \neq m}\left\langle s_{q k} \widetilde{w}_{q k}\right\rangle\left\langle\phi_{k}\right\rangle\right)
$$

are like fixed pseudo-data and

$$
\alpha_{m}=\sum_{q=1}^{Q} \frac{\left\langle s_{q m} \widetilde{w}_{q m}^{2}\right\rangle}{\sigma_{q}^{2}}
$$

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 $q\left(\boldsymbol{\phi}_{m}\right)$ and then continue with other variational EM updates.

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

Consider a single-output regression model:

$$
p(\mathbf{y}, \widetilde{\mathbf{w}}, \mathbf{s})=\mathcal{N}\left(\mathbf{y} \mid \sum_{m=1}^{M} s_{m} \widetilde{w}_{m} \mathbf{x}_{m}, \sigma^{2} \mathbf{I}\right) \prod_{m=1}^{M}\left[\mathcal{N}\left(\widetilde{w}_{m} \mid 0, \sigma_{w}^{2}\right)\left[\pi^{s_{m}}(1-\pi)^{1-s_{m}}\right]\right]
$$

The paired Gibbs sampler iteratively samples from the following conditional

$$
p\left(\widetilde{w}_{m}, s_{m} \mid \widetilde{w}_{\backslash m}, s_{\backslash m}, \mathbf{y}\right)=p\left(\widetilde{w}_{m} \mid s_{m}, \widetilde{w}_{\backslash m}, s_{\backslash m}, \mathbf{y}\right) p\left(s_{m} \mid \widetilde{w}_{\backslash m}, s_{\backslash m}, \mathbf{y}\right)
$$

$p\left(s_{m}=1 \mid \widetilde{w}_{\backslash m}, s_{\backslash m}, \mathbf{y}\right)$ is obtained analytically to be

$$
\begin{aligned}
p\left(s_{m}=1 \mid \widetilde{w}_{\backslash m}, s_{\backslash m}, \mathbf{y}\right) & =\frac{\pi \mathcal{N}\left(\mathbf{y} \mid \sum_{k \neq m} s_{k} \widetilde{w}_{k} \mathbf{x}_{k}, \sigma^{2} \mathbf{I}+\sigma_{w}^{2} \mathbf{x}_{k} \mathbf{x}_{k}^{\mathrm{T}}\right)}{\pi \mathcal{N}\left(\mathbf{y} \mid \sum_{k \neq m} s_{k} \widetilde{w}_{k} \mathbf{x}_{k}, \sigma^{2} \mathbf{I}+\sigma_{w}^{2} \mathbf{x}_{k} \mathbf{x}_{k}^{\mathrm{T}}\right)+(1-\pi) \mathcal{N}\left(\mathbf{y} \mid \sum_{k \neq m} s_{k} \widetilde{w}_{k} \mathbf{x}_{k}, \sigma^{2} \mathbf{I}\right)} \\
& =\frac{\pi \mathcal{N}\left(\mathbf{y} \mid \mathbf{b}_{m}, \sigma^{2} \mathbf{I}+\sigma_{w}^{2} \mathbf{x}_{k} \mathbf{x}_{k}^{\mathrm{T}}\right)}{\pi \mathcal{N}\left(\mathbf{y} \mid \mathbf{b}_{m}, \sigma^{2} \mathbf{I}+\sigma_{w}^{2} \mathbf{x}_{k} \mathbf{x}_{k}^{\mathrm{T}}\right)+(1-\pi) \mathcal{N}\left(\mathbf{y} \mid \mathbf{b}_{m}, \sigma^{2} \mathbf{I}\right)}
\end{aligned}
$$

where

$$
\mathbf{b}_{m}=\sum_{k \neq m} s_{k} \widetilde{w}_{k} \mathbf{x}_{k}
$$

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

$$
p\left(s_{m}=1 \mid \widetilde{w}_{\backslash m}, s_{\backslash m}, \mathbf{y}\right)=\sigma\left(u_{m}\right)
$$

where $\sigma\left(u_{m}\right)=\frac{1}{1+e^{-u_{m}}}$ and

$$
\begin{aligned}
u_{m} & =\log \frac{\pi}{1-\pi}+\frac{1}{2} \log \frac{\sigma^{2}}{\sigma_{w}^{2}}-\frac{1}{2} \log \left(\mathbf{x}_{m}^{\mathrm{T}} \mathbf{x}_{m}+\frac{\sigma^{2}}{\sigma_{w}^{2}}\right)+\frac{1}{2 \sigma^{2}} \frac{\left(\mathbf{x}_{m}^{\mathrm{T}} \mathbf{y}-\sum_{k \neq m} s_{k} \widetilde{w}_{k} \mathbf{x}_{m}^{\mathrm{T}} \mathbf{x}_{k}\right)^{2}}{\left(\mathbf{x}_{m}^{\mathrm{T}} \mathbf{x}_{m}+\frac{\sigma^{2}}{\sigma_{w}^{2}}\right)} \\
& =\log \frac{\pi}{1-\pi}+\frac{1}{2} \log \frac{\sigma^{2}}{\sigma_{w}^{2}}-\frac{1}{2} \log \left(\mathbf{x}_{m}^{\mathrm{T}} \mathbf{x}_{m}+\frac{\sigma^{2}}{\sigma_{w}^{2}}\right)+\frac{1}{2 \sigma^{2}} \frac{\left(\mathbf{x}_{m}^{\mathrm{T}} \mathbf{y}-\mathbf{x}_{m}^{\mathrm{T}} \mathbf{b}_{k}\right)^{2}}{\left(\mathbf{x}_{m}^{\mathrm{T}} \mathbf{x}_{m}+\frac{\sigma^{2}}{\sigma_{w}^{2}}\right)}
\end{aligned}
$$

Also, $p\left(\widetilde{w}_{m} \mid s_{m}=0, \widetilde{w}_{\backslash m}, s_{\backslash m}, \mathbf{y}\right)=\mathcal{N}\left(\widetilde{w}_{m} \mid 0, \sigma_{w}^{2}\right)$ and $p\left(\widetilde{w}_{m} \mid s_{m}=1, \widetilde{w}_{\backslash m}, s_{\backslash m}, \mathbf{y}\right)$ is

$$
p\left(\widetilde{w}_{m} \mid s_{m}=1, \widetilde{w}_{\backslash m}, s_{\backslash m}, \mathbf{y}\right)=\mathcal{N}\left(\widetilde{w}_{m} \left\lvert\, \frac{\mathbf{x}_{m}^{\mathrm{T}} \mathbf{y}-\sum_{k \neq m} s_{k} \widetilde{w}_{k} \mathbf{x}_{m}^{\mathrm{T}} \mathbf{x}_{k}}{\mathbf{x}_{m}^{\mathrm{T}} \mathbf{x}_{m}+\frac{\sigma^{2}}{\sigma_{w}^{2}}}\right., \frac{\sigma^{2}}{\mathbf{x}_{m}^{\mathrm{T}} \mathbf{x}_{m}+\frac{\sigma^{2}}{\sigma_{w}^{2}}}\right)
$$

## References

[1] Iain Murray and Ryan Prescott Adams. Slice sampling covariance hyperparameters of latent Gaussian models. In J. Lafferty, C. K. I. Williams, R. Zemel, J. Shawe-Taylor, and A. Culotta, editors, Advances in Neural Information Processing Systems 23, pages 1723-1731. 2010.
[2] M. Lázaro-Gredilla and M. Titsias. Variational heteroscedastic Gaussian process regression. In 28th International Conference on Machine Learning (ICML-11), pages 841-848, New York, NY, USA, June 2011. ACM.

