Supplementary Material for
Bayesian fMRI Data Analysis with Spatial Basis Function Priors

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1 Derivation of approximate posteriors using Variational Bayes

In this supplementary material we provide the reader with the derivations of the approximate posterior distributions of the spatio-temporal model presented in *Bayesian fMRI Data Analysis with Sparse Spatial Basis Function Priors* by Flandin and Penny. The same notations are used and the reader should refer to this article to have a presentation of the model and the definitions of the variables.

We recall that our generative model is given by

$$\begin{aligned} p(Y, \underbrace{W, \lambda, Z, \alpha, D, S, \pi}_{\Theta}) =& p(Y|W,\lambda)p(\lambda)p(W|Z,\alpha)p(\alpha)p(Z|D,S)p(S)p(D|\pi)p(\pi) \\ =& \left(\prod_{n=1}^{N} p(y_n|w_n,\lambda_n)p(\lambda_n)\right)\left(\prod_{k=1}^{K} p(w_k^T|z_k^T,\alpha_k)p(\alpha_k)\right)\times \\ & \left(\prod_{k=1}^{K}\prod_{l=1}^{L} p(\pi_{kl})\right)\left(\prod_{k=1}^{K}\prod_{l=1}^{L}\prod_{m=1}^{M} p(s_{klm})\right)\times \\ & \left(\prod_{k=1}^{K}\prod_{l=1}^{L}\prod_{n=1}^{N_l} p(z_{kln}|d_{kln},s_{kl})p(d_{kln}|\pi_{kl})\right) \end{aligned} \quad (1)$$

and that we consider the following factorisation for the approximate posterior distribution in the Variational Bayes framework

$$q(\Theta|Y) = \left(\prod_{k=1}^{K} q(z_k^T)q(\alpha_k)\right)\left(\prod_{n=1}^{N} q(w_n)q(\lambda_n)\right)\left(\prod_{k=1}^{K}\prod_{l=1}^{L} q(\pi_{kl})\right)\times \left(\prod_{k}^{K}\prod_{l=1}^{L}\prod_{m}^{M} q(s_{klm}))\right)\left(\prod_{k}^{K}\prod_{l=1}^{L}\prod_{n=1}^{N_l} q(d_{kln})\right) \quad (2)$$

The detailed computations consist, for each subset of parameters θ_i to compute $I(\theta_i)$ given by

$$I(\theta_i) = \int q(\theta_{|i}) \log\left[p(Y, \theta)\right] d\theta_{|i} \quad (3)$$

and recognize the corresponding approximate posterior distribution

$$q(\theta_i) \propto \exp\left[I(\theta_i)\right] \quad (4)$$

which must be of a known form as we chose conjugate priors.

Results presented here are obtained while considering any basis set V. Using an orthonormal basis set, i.e. $V^T V = I_T$, yields further simplifications that are also displayed here. These latter formulae are the ones presented in the article.

1.1 Regression coefficients

The relevant integral for the regression coefficients is

$$I(w_n) = \int q(\lambda_n)q(Z)q(\alpha)q(w_{|n}) \log\left[p(y_n|w_n, \lambda_n)p(W|Z, \alpha)\right] d\lambda_n dZ d\alpha dw_{|n}$$

where

$$\log p(y_n|w_n, \lambda_n) = -\frac{\lambda_n}{2}(w_n^T X^T X w_n - 2w_n^T X^T y_n) + \cdots$$

The prior of W factorises over regressors only while the posterior factorises over voxels. The prior then needs to be rewritten to make appear w_n

$$\begin{aligned}\log p(W|Z,\alpha) &= -\frac{1}{2}\sum_{k=1}^{K}\alpha_k(w_k w_k^T - 2w_k V z_k^T) + \cdots \\ &= -\frac{1}{2}\sum_{n=1}^{N}\left(w_n^T \texttt{diag}(\alpha) w_n - 2w_n^T r_n^T\right) + \cdots \\ &= -\frac{1}{2}\left(w_n^T \texttt{diag}(\alpha) w_n - 2w_n^T r_n^T\right) + \cdots\end{aligned}$$

The integral can then be written as

$$I(w_n) = -\frac{1}{2}w_n^T(\bar{\lambda}_n X^T X + \texttt{diag}(\bar{\alpha}))w_n + w_n^T(\bar{\lambda}_n X^T y_n + \bar{r}_n^T) + \cdots$$

where $\bar{R}$ is a $N \times K$ matrix whose columns contain the top-down predictions of the w_k's

$$\bar{R} = \begin{bmatrix} \vdots & \vdots & & \vdots \\ \bar{\alpha}_1 V \bar{z}_1^T & \bar{\alpha}_2 V \bar{z}_2^T & \cdots & \bar{\alpha}_K V \bar{z}_K^T \\ \vdots & \vdots & & \vdots \end{bmatrix} = \begin{bmatrix} \bar{r}_1 \\ \vdots \\ \bar{r}_N \end{bmatrix} \quad (5)$$

We recognise the logarithm of a Gaussian distribution and we can identify its moments

$$q(w_n|Y) = N(w_n; \bar{w}_n, \Sigma_{w_n}) \quad (6)$$

$$\begin{aligned}\bar{w}_n &= \Sigma_{w_n}\left(\bar{\lambda}_n X^T y_n + \bar{r}_n^T\right) \\ \Sigma_{w_n} &= \left(\bar{\lambda}_n X^T X + \texttt{diag}(\bar{\alpha})\right)^{-1} \quad (7)\end{aligned}$$

1.2 Wavelet coefficients

The relevant integral for the wavelet coefficients is

$$I(z_k^{dT}) = \int q(d_k)q(s_k)q(\alpha_k)q(w_k^T)\log\left[p(w_k^T|z_k^T,\alpha_k)p(z_k^{dT}|d_k,s_k)\right]dw_k^T d\alpha_k ds_k dd_k$$

where

$$\begin{aligned}\log p(w_k^T|z_k^T,\alpha_k) &= -\frac{\alpha_k}{2}(z_k V^T V z_k^T - 2z_k V^T w_k^T) + \cdots \\ &= -\frac{\alpha_k}{2}(z_k^d V_d^T V_d z_k^{dT} - 2z_k^d V_d^T w_k^T) + \cdots\end{aligned}$$

This last equation is true as long as detail levels basis set V_d and coarse levels basis set V_c are orthogonal, i.e. $V_c^T V_d$ is a null matrix.

$$\begin{aligned}\log p(z_k^{dT}|d_k, s_k) &= -\frac{1}{2}\sum_{l=1}^{L}\sum_{n=1}^{N_l}\sum_{m=1}^{M} d_{klnm} s_{klm} z_{kln}^2 + \cdots \\ &= -\frac{1}{2}\sum_{m=1}^{M} z_k \Lambda_{km} z_k^T + \cdots\end{aligned}$$

where

$$\begin{aligned}\Lambda_{km} &= \texttt{blkdiag}(s_{k1m}\Gamma_{k1m}, \ldots, s_{kLm}\Gamma_{kLm}) \\ \Gamma_{klm} &= \texttt{diag}(d_{kl1m}, \ldots, d_{klN_lm})\end{aligned}$$

The integral can then be written as

$$I(z_k^{dT}) = -\frac{1}{2} z_k^d \left(\bar{\alpha}_k V_d^T V_d + \sum_{m=1}^{M} \bar{\Lambda}_{km} \right) z_k^{dT} + z_k^d \bar{\alpha}_k V_d^T \bar{w}_k^T + \cdots$$

with

$$\bar{\Lambda}_{km} = \texttt{blkdiag}(\bar{s}_{k1m}\bar{\Gamma}_{k1m}, \ldots, \bar{s}_{kLm}\bar{\Gamma}_{kLm}) \tag{8}$$

$$\bar{\Gamma}_{klm} = \texttt{diag}(\gamma_{kl1m}, \ldots, \gamma_{klN_lm}) \tag{9}$$

The posterior distribution of z_k then follows a Gaussian law

$$q(z_k^{dT}) = N(z_k^{dT}; \bar{z}_k^{dT}, \Sigma_{z_k^d}) \tag{10}$$

with

$$\bar{z}_k^{dT} = \Sigma_{z_k^d} \bar{\alpha}_k V_d^T \bar{w}_k^T$$

$$\Sigma_{z_k^d} = \left(\bar{\alpha}_k V_d^T V_d + \sum_{m=1}^{M} \bar{\Lambda}_{km} \right)^{-1} \tag{11}$$

With an orthonormal basis set, we have $V_d^T V_d = I_{N_d}$ and the posterior variance-covariance matrix $\Sigma_{z_k^d}$ becomes diagonal

$$\Sigma_{z_k^d} = \text{diag}(\sigma_{z_{kln}}^2)$$

which leads to a new factorisation of the posterior wavelet coefficients distribution over wavelet levels and wavelet coefficients in each level

$$q(z_k^{dT}) = \prod_{l=1}^{L} \prod_{n=1}^{N_l} q(z_{kln}) = \prod_{l=1}^{L} \prod_{n=1}^{N_l} N(z_{kln}; \bar{z}_{kln}, \sigma^2_{z_{kln}}) \tag{12}$$

where

$$\begin{aligned} \sigma^2_{z_{kln}} &= \left(\bar{\alpha}_k + \sum_{m=1}^{M} \bar{s}_{klm} \gamma_{klnm} \right)^{-1} \\ \bar{z}_{kln} &= \frac{\bar{\alpha}_k V_{ln}^T \bar{w}_k^T}{\bar{\alpha}_k + \sum_{m=1}^{M} \bar{s}_{klm} \gamma_{klnm}} \end{aligned} \tag{13}$$

where V_{ln}^T is the basis for nth element of lth detail level of the wavelet transform V.

1.3 Wavelet coefficient switches

The relevant integral for the wavelet coefficient switches is

$$I(d_{kln}) = \int q(z_{kln}) q(s_{kl}) q(\pi_{kl}) \log \left[p(z_{kln}|d_{kln}, s_{kl}) p(d_{kln}|\pi_{kl}) \right] dz_{kln} ds_{kl} d\pi_{kl}$$

where

$$\log p(z_{kln}|d_{kln}, s_{kl}) = \sum_{m=1}^{M} d_{klnm} \left(\frac{1}{2} \log s_{klm} - \frac{s_{klm}}{2} z_{kln}^2 \right) + \cdots$$

$$\log p(d_{kln}|\pi_{kl}) = \sum_{m=1}^{M} d_{klnm} \log \pi_{klm} + \cdots$$

We then obtain

$$\begin{aligned} I(d_{kln}) &= \sum_{m=1}^{M} d_{klnm} \left[\frac{1}{2} \int q(s_{klm}) \log s_{klm} ds_{klm} - \frac{\bar{s}_{klm}}{2} (\bar{z}_{kln}^2 + \sigma^2_{z_{kln}}) + \int q(\pi_{klm}) \log \pi_{klm} d\pi_{klm} \right] + \cdots \\ &= \sum_{m=1}^{M} d_{klnm} \left[\frac{1}{2} \log \tilde{s}_{klm} - \frac{1}{2} \bar{s}_{klm} (\bar{z}_{kln}^2 + \sigma^2_{z_{kln}}) + \log \tilde{\pi}_{klm} \right] + \cdots \\ &= \sum_{m=1}^{M} d_{klnm} \log \left[\tilde{s}_{klm}^{1/2} \tilde{\pi}_{klm} \exp \left(-\frac{\bar{s}_{klm}}{2} (\bar{z}_{kln}^2 + \sigma^2_{z_{kln}}) \right) \right] + \cdots \end{aligned}$$

with

$$\log \tilde{\pi}_{klm} = \int q(\pi_{klm}) \log \pi_{klm} d\pi_{klm} \quad \text{and} \quad \log \tilde{s}_{klm} = \int q(s_{klm}) \log s_{klm} ds_{klm} \tag{14}$$

We can then conclude that d_{kln} follows a Multinomial distribution

$$q(d_{kln}) = Mult(d_{kln}; \gamma_{kln}) \tag{15}$$

where

$$\gamma_{klnm} = \frac{\tilde{\gamma}_{klnm}}{\sum_{m'} \tilde{\gamma}_{klnm'}} \quad \text{and} \quad \tilde{\gamma}_{klnm} = \tilde{\pi}_{klm} \tilde{s}_{klm}^{1/2} \exp\left(-\frac{\bar{s}_{klm}}{2}(\bar{z}_{kln}^2 + \sigma_{z_{kln}}^2)\right) \tag{16}$$

1.4 Mixing proportions

The relevant integral for the mixing proportions is

$$I(\pi_{kl}) = \int q(d_{kln}) \log \left[\prod_{n=1}^{N_l} p(d_{kln}|\pi_{kl}) p(\pi_{kl})\right] dd_{kln}$$

where

$$\log p(\pi_{kl}) = \sum_{m=1}^{M} (f_{0m} - 1) \log \pi_{klm} + \cdots$$

$$\log \prod_{n=1}^{N_l} p(d_{kln}|\pi_{kl}) = \sum_{n=1}^{N_l} \sum_{m=1}^{M} d_{klnm} \log \pi_{klm} + \cdots$$

This gives

$$\begin{aligned} I(\pi_{kl}) &= \sum_{m=1}^{M} \left[(f_{0m} - 1) \log \pi_{klm} + \sum_{n=1}^{N_l} \gamma_{klnm} \log \pi_{klm}\right] + \cdots \\ &= \sum_{m=1}^{M} \log \left(\pi_{klm}^{f_{0m} + \bar{N}_{klm} - 1}\right) + \cdots \end{aligned}$$

where

$$\bar{N}_{klm} = \sum_{n=1}^{N_l} \gamma_{klnm} \tag{17}$$

Then π_{kl} follows a Dirichlet distribution

$$q(\pi_{kl}) = Dir(\pi_{kl}; f_{kl}) \tag{18}$$

where

$$f_{klm} = \bar{N}_{klm} + f_{0m} \tag{19}$$

and in particular, we have the following result

$$\log \tilde{\pi}_{klm} = \int q(\pi_{klm}) \log \pi_{klm} d\pi_{klm} = \Psi(f_{klm}) - \Psi\left(\sum_{m'=1}^{M} f_{klm'}\right) \tag{20}$$

1.5 Noise precisions

The relevant integral for the noise precisions is

$$I(\lambda_n) = \int q(w_n) \log \left[p(y_n|w_n, \lambda_n)p(\lambda_n)\right] dw_n$$

where

$$\log p(y_n|w_n, \lambda_n) = \frac{T}{2} \log \lambda_n - \frac{\lambda_n}{2}(y_n - Xw_n)^T(y_n - Xw_n) + \cdots$$

$$\log p(\lambda_n) = (c_{\lambda_0} - 1) \log \lambda_n - \frac{\lambda_n}{b_{\lambda_0}} + \cdots$$

Then

$$\begin{aligned} I(\lambda_n) &= \frac{T}{2} \log \lambda_n - \frac{\lambda_n}{2}\left[(y_n - X\bar{w}_n)^T(y_n - X\bar{w}_n) + \mathtt{tr}(\Sigma_{w_n} X^T X)\right] + (c_{\lambda_0} - 1) \log \lambda_n - \frac{\lambda_n}{b_{\lambda_0}} + \cdots \\ &= \left(\frac{T}{2} + c_{\lambda_0} - 1\right) \log \lambda_n - \lambda_n \left[\frac{1}{2}\left[(y_n - X\bar{w}_n)^T(y_n - X\bar{w}_n) + \mathtt{tr}(\Sigma_{w_n} X^T X)\right] + \frac{1}{b_{\lambda_0}}\right] + \cdots \end{aligned}$$

from which we conclude that λ_n follows a Gamma distribution

$$q(\lambda_n) = G_a(\lambda_n; b_{\lambda_n}, c_{\lambda_n}) \tag{21}$$

with

$$\begin{aligned} \frac{1}{b_{\lambda_n}} &= \frac{1}{2}\left[(y_n - X\bar{w}_n)^T(y_n - X\bar{w}_n) + \mathtt{tr}(\Sigma_{w_n} X^T X)\right] + \frac{1}{b_{\lambda_0}} \\ c_{\lambda_n} &= \frac{T}{2} + c_{\lambda_0} \end{aligned} \tag{22}$$

The expectation of λ_n is given by $\bar{\lambda}_n = b_{\lambda_n} c_{\lambda_n}$.

1.6 Wavelet residual precisions

The relevant integral for the wavelet residual precisions is

$$I(\alpha_k) = \int q(z_k^T) q(w_k^T) \log \left[p(w_k^T | z_k^T, \alpha_k) p(\alpha_k) \right] dw_k^T dz_k^T$$

where

$$\log p(w_k^T | z_k^T, \alpha_k) = \frac{N}{2} \log \alpha_k - \frac{\alpha_k}{2} \left(w_k^T - V z_k^T \right)^T \left(w_k^T - V z_k^T \right) + \cdots$$

$$\log p(\alpha_k) = -\frac{\alpha_k}{b_{\alpha_0}} + (c_{\alpha_0} - 1) \log \alpha_k + \cdots$$

This gives

$$\begin{aligned} I(\alpha_k) = & \left(\frac{N}{2} + c_{\alpha_0} - 1 \right) \log \alpha_k - \frac{\alpha_k}{b_{\alpha_0}} \\ & - \frac{\alpha_k}{2} \left[(\bar{w}_k^T - V \bar{z}_k^T)^T (\bar{w}_k^T - V \bar{z}_k^T) + \texttt{tr}(\Sigma_{w_k}) + \texttt{tr}(V_d^T V_d \Sigma_{z_k^d}) \right] + \cdots \end{aligned}$$

where we recognise a Gamma distribution

$$q(\alpha_k) = G_a(\alpha_k; b_{\alpha_k}, c_{\alpha_k}) \tag{23}$$

with

$$\begin{aligned} \frac{1}{b_{\alpha_k}} &= \frac{1}{2} \left[\texttt{tr}(\Sigma_{w_k}) + \texttt{tr}(V_d^T V_d \Sigma_{z_k^d}) + (\bar{w}_k^T - V \bar{z}_k^T)^T (\bar{w}_k^T - V \bar{z}_k^T) \right] + \frac{1}{b_{\alpha_0}} \\ c_{\alpha_k} &= \frac{N}{2} + c_{\alpha_0} \end{aligned} \tag{24}$$

If we consider an orthonormal basis set V, there are further simplifications and one of the trace terms in the update equations becomes

$$\texttt{tr}(V_d^T V_d \Sigma_{z_k^d}) = \sum_{l=1}^{L} \sum_{n=1}^{N_l} \sigma_{z_{kln}^2}$$

The expectation of α_k is given by $\bar{\alpha}_k = b_{\alpha_k} c_{\alpha_k}$.

1.7 Wavelet coefficient precisions

The relevant integral for the wavelet coefficient precisions is

$$I(s_{klm}) = \int q(z_{kl})q(d_{klm}) \log \left[\prod_{n=1}^{N_l} p(z_{kln}|d_{klnm}, s_{klm})p(s_{klm}) \right] dz_{kl} dd_{klm}$$

where

$$\log \prod_{n=1}^{N_l} p(z_{kln}|d_{klm}, s_{klm}) = -\frac{1}{2} s_{klm} z_{kl} \, \mathtt{diag}(d_{kl1m}, \ldots, d_{klN_l m}) z_{kl}^T + \frac{\sum_{n=1}^{N_l} d_{klnm}}{2} \log s_{klm} + \cdots$$

$$\log p(s_{klm}) = (c_{s_0} - 1) \log s_{klm} - \frac{s_{klm}}{b_{s_0}} + \cdots$$

This yields

$$\begin{aligned} I(s_{klm}) = & -\frac{1}{2} s_{klm} \left(\bar{z}_{kl} \bar{\Gamma}_{klm} \bar{z}_{kl}^T + \mathtt{tr}(\bar{\Gamma}_{klm} \Sigma_{z_{kl}}) \right) \\ & + \frac{\sum_{n=1}^{N_l} \gamma_{klnm}}{2} \log s_{klm} + (c_{s_0} - 1) \log s_{klm} - \frac{s_{klm}}{b_{s_0}} + \cdots \end{aligned}$$

and again we recognise a Gamma distribution

$$q(s_{klm}) = G_a(s_{klm}; b_{s_{klm}}, c_{s_{klm}}) \tag{25}$$

with

$$\begin{aligned} \frac{1}{b_{s_{klm}}} &= \frac{1}{2} \left[\mathtt{tr}(\bar{\Gamma}_{klm} \Sigma_{z_{kl}}) + \bar{z}_{kl} \bar{\Gamma}_{klm} \bar{z}_{kl}^T \right] + \frac{1}{b_{s_0}} \\ c_{s_{klm}} &= \frac{\bar{N}_{klm}}{2} + c_{s_0} \text{ and } \bar{N}_{klm} = \sum_{n=1}^{N_l} \gamma_{klnm} \end{aligned} \tag{26}$$

With an orthonormal wavelet basis set, there are further simplifications

$$\frac{1}{b_{s_{klm}}} = \frac{1}{2} \left[\sum_{n=1}^{N_l} \gamma_{klnm} (\sigma_{z_{kln}}^2 + \bar{z}_{kln}^2) \right] + \frac{1}{b_{s_0}}$$

The expectation of s_{klm} is given by $\bar{s}_{klm} = b_{s_{klm}} c_{s_{klm}}$. We also have the following result

$$\log \tilde{s}_{klm} = \int q(s_{klm}) \log s_{klm} ds_{klm} = \Psi(c_{s_{klm}}) + \log b_{s_{klm}} \tag{27}$$