Variational Laplace in Generalised Coordinates for Spectral Dynamic Causal Modelling

Alexander D. Shaw
Computational Psychiatry and Neuropharmacology Systems Lab
University of Exeter, UK
a.d.shaw@exeter.ac.uk

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Abstract

This document describes a variational Laplace (VL) optimisation scheme for Dynamic Causal Modelling (DCM) in the frequency domain, extended to operate in generalised coordinates of spectral data. The method provides a computationally efficient alternative to full generalised filtering, while preserving key benefits such as derivative-informed data fitting and smoother spectral gradients. The full mathematical formulation is presented for direct implementation.

1 Introduction

Dynamic Causal Modelling (DCM) has become a widely used framework for estimating biophysically interpretable neural parameters from electrophysiological data. For spectral DCM, model inversion typically relies on Variational Laplace (VL) under a Gaussian (Laplace) approximation to the posterior. Here we present an extension of VL that incorporates *generalised coordinates* of observation in the frequency domain, providing a principled way to include frequency derivatives of spectral data in the inversion. This enhances sensitivity to spectral shape, curvature, and peak structure, thereby improving model inversion robustness.

The approach retains the standard DCM prior structure, but augments the data-fit term using generalised spectral transforms. Optimisation is performed using a Gauss–Newton scheme with Levenberg–Marquardt damping, alongside free energy-based acceptance and likelihood annealing for stability.

2 Generative Model

Let $y \in \mathbb{R}^{F\times C}$ denote the observed (cross-)spectral data at frequencies $f = \{f_1, \ldots, f_F\}$, with C channels or components. The DCM generative model specifies predicted spectra $g(\theta)$ as a function of neural and observation parameters θ:

$$y = g(\theta) + \varepsilon, \qquad \varepsilon \sim \mathcal{N}(0, \Pi_y^{-1}), \tag{1}$$

where Π_y is the (diagonal) observation precision matrix. A Gaussian prior is placed over parameters:

$$\theta \sim \mathcal{N}(\mu, \Pi_\theta^{-1}), \tag{2}$$

with prior mean μ and prior precision Π_θ.

3 Generalised Coordinates of Spectral Data

To incorporate smoothness and spectral-derivative information, we transform the data into *generalised coordinates* across frequency. For generalised order $k = 0, \ldots, K$, define:

$$\phi_k(f) = (i2\pi f)^k. \tag{3}$$

We then construct a stacked generalised observation vector:

$$\tilde{y} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_K \end{bmatrix}, \qquad y_k = W \cdot \mathrm{Re}[\log(y) \odot \phi_k(f)], \tag{4}$$

where $\odot$ denotes elementwise multiplication, W is a frequency-weighting matrix (allowing band-specific weighting), and $\mathrm{Re}[\cdot]$ extracts the real part.

The same transformation is applied to the model prediction:

$$\tilde{g}(\theta) = \begin{bmatrix} g_0(\theta) \\ g_1(\theta) \\ \vdots \\ g_K(\theta) \end{bmatrix}. \tag{5}$$

Thus, model inversion is performed not on y directly, but on its generalised-coordinate representation $\tilde{y}$.

4 Free Energy Objective

We seek the Maximum A Posteriori (MAP) estimate:

$$\hat{\theta} = \arg\max_\theta \mathcal{F}(\theta), \tag{6}$$

where the negative variational free energy (up to additive constants) is:

$$\mathcal{F}(\theta) = -\frac{1}{2}\beta \, \|\tilde{y} - \tilde{g}(\theta)\|^2 - \frac{1}{2}(\theta - \mu)^\top \Pi_\theta (\theta - \mu). \tag{7}$$

Here, $\beta \in (0, 1]$ acts as an annealing factor that gradually increases the contribution of the likelihood term during optimisation.

5 Gauss–Newton Update in Generalised Coordinates

Let $J(\theta)$ denote the Jacobian of the generalised-coordinate model prediction:

$$J(\theta) = \frac{\partial \tilde{g}(\theta)}{\partial \theta}. \tag{8}$$

The gradient of the free energy is:

$$\nabla_\theta \mathcal{F}(\theta) = -\beta\, J(\theta)^\top (\tilde{y} - \tilde{g}(\theta)) - \Pi_\theta(\theta - \mu), \tag{9}$$

and the Gauss–Newton approximation to the Hessian is:

$$G(\theta) = \beta\, J(\theta)^\top J(\theta) + \Pi_\theta. \tag{10}$$

For numerical stability, we employ a Levenberg–Marquardt (LM) regularisation:

$$G_\lambda(\theta) = G(\theta) + \lambda I, \tag{11}$$

with damping parameter $\lambda > 0$ adapted during the optimisation.

The update step is:

$$\delta\theta = -G_\lambda(\theta)^{-1}\, \nabla_\theta \mathcal{F}(\theta), \qquad \theta \leftarrow \theta + \alpha\, \delta\theta, \tag{12}$$

where α is a trust-region step size.

6 Acceptance, Annealing and Convergence

At each iteration, the free energy is evaluated for the current and proposed parameters. A step is accepted if it increases free energy:

$$\mathcal{F}_{\text{new}} \geq \mathcal{F}_{\text{old}} \quad \Rightarrow \quad \text{accept step, decrease } \lambda,$$

otherwise:

$$\mathcal{F}_{\text{new}} < \mathcal{F}_{\text{old}} \quad \Rightarrow \quad \text{reject step, increase } \lambda.$$

Annealing proceeds over a sequence $\beta_1 < \beta_2 < \cdots < \beta_M = 1$, for example $\beta = [0.1, 0.3, 0.6, 1.0]$.

At convergence, the posterior parameter mean and covariance under the Laplace approximation are:

$$\hat{\theta} = \theta^\star, \qquad \Sigma_\theta = G(\theta^\star)^{-1}. \tag{13}$$

7 Conclusion

This generalised-coordinate VL scheme provides a lightweight alternative to full generalised filtering for spectral DCM, while capturing higher-order frequency-domain structure. It is computationally efficient, stable, and compatible with existing DCM implementations that expose

a frequency-domain observation operator.