# Supplementary material

# *Jafarian A, Zeidman P, Litvak V and Friston K, Structure Learning in Coupled Dynamical Systems and Dynamic Causal Modelling, Philosophical Transactions A, DOI: 10.1098/rsta.2019.0048.*

This brief note explains the parameter estimation routine in DCM. Detailed explanation can be found in (1,2). A generic form of a nonlinear model with unknown parameter vector is as follows:

|  |  |  |
| --- | --- | --- |
|  |  | (A1) |

In equation (A1), is an additive error term with Gaussian distribution (where is a covariance matrix). The inverse of the error covariance matrix is called the precision matrix and is denoted by . The precision matrix can be decomposed using known precision basis functions as follows:

|  |  |  |
| --- | --- | --- |
|  |  |  (A2) |

In equation (A2), scalar is called a hyperparameter (since it is used to define the distribution of the error term) and is the number of the precision component. The aim of model *inversion* is to infer the posterior probability of parameters and hyperparameters given their (normal) prior densities which are denoted by and, respectively. An iterative optimisation scheme is used in DCM that searches for settings of the parameters that maximise the log model evidence (1,2). However, since in practice the log model evidence cannot be computed exactly, and an approximation called the negative variational free energy functional (or evidence lower bound) is used and is returned by DCM. The negative variational free energy, hereafter the free energy, is used as the basis for comparing the evidence for different candidate models (Bayesian model selection).

The scheme for estimation of model parameters in DCM is called variational Bayes method under Laplace approximation (a.k.a, variational Laplace), and is employed to approximate posterior densities of parameters with Gaussian distributions. The approximation can be evaluated in terms of the difference ( divergence) between the true posterior and the approximated Gaussian posterior over the parameters. However, since the true posterior is not known, the difference cannot be computed directly, and the goodness of the approximation needs to be evaluated indirectly through optimisation of the free energy. This follows because the log model evidence can be expressed as the algebraic sum of the negative free energy and the KL divergence, given in Equation 2 of the main text and re-expressed here for convenience:

|  |  |  |
| --- | --- | --- |
|  |  | (A3) |

As the left hand side of this equation - the log model evidence – is a fixed value, maximising the free energy will minimize the difference between the approximate and true parameter densities.

Estimation of the densities in DCM rests upon a mean field approximation, meaning that probability densities over the parameters and hyperparameters are treated as independent and can therefore be factorised. The posterior density over the parameters factorise as follows:

|  |  |  |
| --- | --- | --- |
|  |  | (A4) |

This allows estimation of parameters and hyperparameters to be carried out separately. Under the mean field approximation, the free energy functional can be written as follows:

|  |  |  |
| --- | --- | --- |
|  |  | (A5) |

In DCM, to calculate the free energy in equation (A5), the function is approximated around the estimated posterior mean of unknown parameters using a second order Taylor series expansion - formally known as a Laplace approximation (1). In effect, equation (A5) can be expressed in a closed form (i.e., analytically) in terms of Gaussian functions.

To find the posterior density over the parameters, iterative maximization of the Laplace approximation of the following energy integrals is performed by the DCM software:

|  |  |  |
| --- | --- | --- |
|  |  | (A6) |

In equation (A6), is the likelihood function. During the ensuing iterations, the posterior mean of the parameters (in the same way for hyperparameters) are updated using the following rule:

|  |  |  |
| --- | --- | --- |
|  |  | (A7) |

In the equation (A7), is the step size for updates to the model parameters. This is defined as where and are the gradient () and Hessian ( ) of the free energy functional. In effect, equation (A7) resembles a Newton update method. Intuitively, in the region that the gradient changes slowly, changes to the parameters are large to avoid an unnecessary search, making the proposed algorithm efficient. The posterior covariance of the parameters is defined as negative inverse curvature (for hyperparameters ). The estimation scheme iterates over the parameters and hyperparameters until the free energy quantity ceases to change significantly.

Reference

1. Friston K, Mattout J, Trujillo-Barreto N, Ashburner J, Penny W, Friston K. Variational free energy and the Laplace approximation. Neuroimage. 2006 Jan 1;34(1):220–34.

2. Friston KJ, Trujillo-Barreto N, Daunizeau J. DEM: A variational treatment of dynamic systems. Neuroimage. 2008;41(3):849–85.