

Toolbox ‘BMMSB’

This manual aims to show detailed guidelines on using our toolbox, including the usage of primary functions, our settings of initial values, and a control panel for reproducing our simulation results. All functions are written in a form that can be easily used on computing clusters.

BMMSB_ContPnl_ms.m

An example of our toolbox ‘BMMSB’

Description:

The Control Panel of our proposed Bayesian method with the mixed-membership stochastic blockmodel prior (BMMSB).

This Control Panel serves as an example of analyzing data using our toolbox. It is written as a function that can be easily modified to use on computing clusters. Users can use this control panel to reproduce the results in our simulation studies (Section 4) and modify this file to analyze their data without difficulty.

Details:

This control panel shows a step-by-step procedure to analyze the 1000 subjects’ simulated data in our simulation studies (Section 4). Due to the large file size, our toolbox does not include the simulated time series but the true network structure contained in *BMMSB_A_true_S.mat*. Therefore, users can first generate the same simulated data as we analyzed in our paper through the function *BMMSB_generate_Simu.m*, then use this control panel to reproduce our results.

The control panel also includes the calculation of the true positive rate (TPR), the false positive rate (FPR), and the area under the curve (AUC) that we presented in our simulation studies, given our variational Bayesian algorithm’s outputs and the true network structure.

BMMSB_VB_par_ms.m *The variational Bayesian algorithm for estimating our proposed Bayesian model*

Description:

This is the primary function of our variational Bayesian algorithm, which is developed for estimating our proposed Bayesian model. The function incorporates parallel computing, which can significantly reduce the computation time.

Usage:

```
[A_Gam_alpha, A_Gam_u, A_Gam_w, m_phi, p_iota, E_log_B, E_log_1_B, KL]
= BMMSB_VB_par_ms(X_S, mite, A_Gam_alpha0, A_Gam_u0, A_Gam_w0, m_phi0, p_iota0,
  E_log_B, E_log_1_B, xi_sq0, l0, u0)
```

Input:

X_S	The estimated state functions (treated as given data) of multiple scans
mite	The max expected number of iterations (default is 20)
l0, u0	Hyperparameters in \mathbf{B} 's prior
xi_sq0	Hyperparameter in $\mathbf{A}^{s,l}$'s prior
A_Gam_alpha0, A_Gam_u0, A_Gam_w0	Initial values of Φ_{ij}^s s
m_phi0	Initial values of Φ^{m_i} s
p_iota0	Initial values of Φ^{p_i} s
E_log_B, E_log_1_B	Initial values of $\mathbb{E}_{q_4(\mathbf{B}_{k_1 k_2})}[\log \mathbf{B}_{k_1 k_2}]$ and $\mathbb{E}_{q_4(\mathbf{B}_{k_1 k_2})}[\log(1 - \mathbf{B}_{k_1 k_2})]$

Output:

A_Gam_alpha, A_Gam_u, A_Gam_w, m_phi, and p_iota are the updated values of Φ_{ij}^s , Φ^{m_i} s, and Φ^{p_i} s at the last iteration. E_log_B and E_log_1_B are the evaluated expectations of $\mathbb{E}_{q_4(B_{k_1 k_2})}[\log B_{k_1 k_2}]$ s and $\mathbb{E}_{q_4(B_{k_1 k_2})}[\log(1 - B_{k_1 k_2})]$ s at the last iteration. KL records the KL-divergence values at all iterations.

Details:

The outputs of *BMMSB_VB_par_ms.m* contain the estimated values of the variational parameters and the KL-divergence values at all iterations.

Other functions including *BMMSB_update_m.m*, *BMMSB_update_A_Gam_ms.m*, *BMMSB_update_p.m*, *BMMSB_update_B_kk.m*, *BMMSB_update_B_kl.m* are the updating steps in our variational Bayesian algorithm; *BMMSB_update_E_log_B.m* evaluates $\mathbb{E}_{q_4(B_{k_1 k_2})}[\log B_{k_1 k_2}]$ s and $\mathbb{E}_{q_4(B_{k_1 k_2})}[\log(1 - B_{k_1 k_2})]$ s based on the estimated variational parameters; *BMMSB_KL.m* calculates the KL-divergence.

MARSS_ContPnl.m	<i>The function for estimating state functions through a standard multivariate autoregressive state-space (MARSS) model</i>
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Description:

This is the function for estimating state functions \mathbf{X} through a standard MARSS. Users can estimate the state functions of each subject's different fMRI runs independently using this function.

Details:

MARSS.m uses a MCMC algorithm for the posterior inference of the standard MARSS. Other functions including *MARSS_A.s.m*, *MARSS_X.s.m*, *MARSS_C.s.m*, *MARSS_R.s.m*, *MARSS_mu.s.m* are the updating steps. More details can be found in Li, H., Wang, Y., Yan, G., Sun, Y., Tanabe, S., Liu, C.-C., Quigg, M. S. and Zhang, T. (2021). A Bayesian State-Space Approach to Mapping Directional Brain Networks. *Journal of the American Statistical Association*, 116(536): 1637-1647.

BMMSB_Omega.m

Determining modules and the number of modules

Description:

This function is for the posterior inference (Section 3.1.) It determines modules and the number of modules from the outputs of *BMMSB_VB_par_ms.m*. *BMMSB_P.m* uses the outputs of this function to identify modules in subject-specific and population-mean brain networks.

BMMSB_P.m

Identification of modules

Description:

This function is for the posterior inference (Section 3.1.) It identifies modules in subject-specific and population-mean brain networks. *BMMSB_BIC.m* uses the outputs of this function to calculate the BIC for choosing hyperparameters (Section 3.2).

BMMSB_BIC.m

Calculating BIC

Description:

This function calculates the BIC for choosing hyperparameters (Section 3.2). Users can compare the BIC values of different ξ_0^2 candidates and choose the ξ_0^2 with the smallest BIC.

Description:

This function generates different subjects' simulated data in multiple fMRI runs with a given true network structure. Users can generate the same simulated data as we used in our paper by running this function with the true network structure *BMMSB_A_true_S.m*.

Details:

This function and *BMMSB_spm_fx_fmri.m* are modified from the functions in the following two toolboxes:

SPM12 (<https://www.fil.ion.ucl.ac.uk/spm/software/spm12/>) and rDCM (Frässle, S., Lomakina, E.I., Razi, A., Friston, K.J., Buhmann, J.M., Stephan, K.E., 2017. Regression DCM for fMRI. *NeuroImage*, 155, 406–421. <https://doi.org/10.1016/j.neuroimage.2017.02.090>; Frässle, S., Lomakina, E.I., Kasper, L., Manjaly Z.M., Leff, A., Pruessmann, K.P., Buhmann, J.M., Stephan, K.E., 2018. A Generative Model of Whole-Brain Effective Connectivity. *NeuroImage*, 179, 505–529. <https://doi.org/10.1016/j.neuroimage.2018.05.058>). It also depends on the SPM12 toolbox.

Reference:

Yaotian Wang, Guofen Yan, Xiaofeng Wang, Shuoran Li, Lingyi Peng, Dana L Tudorascu, and Tingting Zhang (2022). A Variational Bayesian Approach to Identifying Whole-Brain Directed Networks with fMRI Data, *The Annals of Applied Statistics*, accepted