cvBMS Toolkit Manual

This manual describes the use of MATLAB code associated with the following publication:

> Soch J, Haynes JD, Allefeld C (2016): "How to avoid mismodelling in GLM-based fMRI data analysis: cross-validated Bayesian model selection", NeuroImage, vol. 141, pp. 469-489. DOI: 10.1016/j.neuroimage.2016.07.047.

If you use this method in published research, please refer to it as "cross-validated Bayesian model selection (cvBMS)" or simply "the cvBMS approach" and cite the paper mentioned above. The cvBMS toolkit is compatible with SPM8 and SPM12, can be obtained from the corresponding author of this publication and is supplied as a ZIP file called "MACS_cvBMS.zip". Internally, this version is referred to as "MACS V13a", "MACS V0.9a" and "Release cvBMS".

Structure of the Toolkit

After download, the ZIP file should be unpacked and added to the MATLAB path. Generally, functions in the toolkit folder are organized into two groups with three sub-groups each:

- *interface functions* – allowing the user to perform desired operations:
  - `MA_*.m` : model assessment
  - `MC_*.m` : model comparison (not included in this limited release)
  - `MS_*.m` : model selection
- *mathematical functions* – allowing the toolkit to perform statistical analysis:
  - `ME_*.m` : model estimation
  - `MD_*.m` : many distributions
  - `MF_*.m` : more functions

Users of the toolkit will only need to call interface functions, but developers are highly encouraged to have a look at and play around with the mathematical functions as well. The cvBMS toolkit requires SPM8 or later running on MATLAB 7.4 or later. No additional MATLAB toolboxes are needed.

Application of the Toolkit

The cvBMS methods are written for general linear models (GLMs) applied to functional magnetic resonance imaging (fMRI) data and directly build on "SPM.mat" files created using Statistical Parametric Mapping (SPM), Versions 8 or 12.

The overall goal of cvBMS is model inference. Therefore, at least two models ($M \geq 2$) have to be fitted to at least one subject ($N \geq 1$). If this has been done, model inference proceeds in two steps: model assessment and model selection.

Step 1: First-level model assessment

In the first step, each model in each subject (i.e. on the first level) is evaluated using the cross-validated log model evidence (cvLME) in each voxel (i.e. voxel-wise). To this end, the following commands have to be executed:

```
>> load [...]\SPM.mat      % loads an SPM.mat
>> MA_cvLME_multi(SPM)     % calculates the cvLME
```

This will produce a voxel-wise cvLME map in the folder where the first-level model corresponding to "SPM.mat" is located, here abbreviated as `[...]`. Note that for this function call, it does not matter

- whether this model is already *estimated* – in case it is not, this is done using `MA_GLM_AR_only`; however, the model must have been *specified* – or
- whether this model is a multi-session GLM or a single-session GLM – in the latter case, the toolkit automatically calls `MA_cvLME_single`.

Step 2: Second-level model selection

In the second step, cvLME maps from all models applied to all subjects (i.e. on the second level) are combined to calculate estimated model frequencies in each voxel (i.e. voxel-wise) by a procedure called random-effects Bayesian model selection (RFX BMS). For this purpose, a MATLAB batch must be created using the SPM Batch Editor. After clicking on "Batch" in the SPM menu window (top left), simply select

- in SPM8: SPM >> Stats >> Bayesian Model Selection >> BMS: Maps; or
- in SPM12: SPM >> Stats >> Bayesian Model Selection >> BMS: Maps (Inference).

Here, it is enough to specify (i) the BMS directory, (ii) the LME maps and (iii) the model names; all other fields can be left as default. Then, this batch has to be saved and the following commands have to be executed:

```
>> load [...]\batch.mat                % loads the SPM batch
>> MS_BMS_group_mods(matlabbatch)      % performs an RFX BMS
```

This will produce voxel-wise estimated frequency maps and exceedance probability maps in the folder that was selected as the BMS directory, ideally the one into which the SPM batch was saved, here abbreviated as `[...]`. Estimated model frequencies come in the form of expected frequencies (EF), i.e. posterior means, and likeliest frequencies (LF), i.e. posterior modes. Exceedance probabilities (EP) quantify the probability that a model is more frequent in the population than any other model, given the data.

(Step 3: Group-level selected-model maps)

When the goal of model selection is methodological control, i.e. identifying the optimal model for data analysis, one is only interested in the model which has the highest EF, LF or EP (all give rise to the same ranking). This is equivalent to creating selected-model maps (SMMs) which can be achieved by executing the following commands:

```
>> load [...]\BMS.mat      % loads a BMS.mat
>> MS_SelMod_BMS(BMS)      % determines SMMs
```

This will produce a sub-folder in the BMS directory, here abbreviated as `[...]`, containing continuous SMMs which report in each voxel (i.e. voxel-wise) whether a model is selected (indicated by non-NaN image values) and its likeliest frequency (where it is selected).

Summary: The cvBMS toolkit pipeline

To facilitate usability of the cvBMS toolkit, the toolkit folder contains a MATLAB script called "cvBMS_Pipeline.m" as a template for cvBMS-style analysis of study data arranged in a subject-model folder hierarchy. This pipeline also includes an optional intermediate "Step 1.5" in which log model evidences (LME) are aggregated into log family evidences (LFE) to quantify model families. For advice on this latter aspect, type `help MA_LFE_uniform` in the MATLAB command window, read the section "First-level Bayesian model inference" of the referenced paper or contact the corresponding author.

Hands-On Example

In this section, we describe a simple example for application of the cvBMS toolkit. Since we don't supply data with our toolkit, we will work with an SPM template data set that can be downloaded from the internet. Because this is a single-subject data set, there is no real second-level analysis. We will however perform a pseudo-second-level analysis with this one subject in order to familiarize the user with all steps of a cvBMS analysis.

Step 0: Pre-processing and model estimation

Please download the SPM8 Manual or SPM12 Manual and work through Chapter 29/31 until the end of Section 29.3/31.3. At this point, you will have pre-processed the data and estimated two first-level GLMs, a "categorical model" and a "parametric model". These models share several similarities and exhibit two differences:

- The categorical model uses two HRF derivatives (time derivative and dispersion derivative) while the parametric model doesn't use HRF derivatives.
- The parametric model includes two parametric modulators in quadratic expansion while the categorical model doesn't use parametric modulators.
- Both models describe four experimental conditions, contain six movement regressors and include one implicit baseline.
- In effect, the categorical model has 19 (= 4 x 3 + 6 + 1) regressors and the parametric model has 15 (= 4 + 2 x 2 + 6 + 1) regressors.

After these preliminary analyses, the categorical model is located in `DIR/categorical` and the parametric model is located in `DIR/parametric` where `DIR` is some folder on your computer.

Step 1: First-level model assessment

Model assessment for these two models can be carried out as follows:

```
>> load DIR/categorical/SPM.mat
>> MA_cvLME_single(SPM)
>> load DIR/parametric/SPM.mat
>> MA_cvLME_single(SPM)
```

After that, a file "MA_cvLME_Ky_11.nii" has been created in each model folder.

Step 2: "Second-level" model selection

Model selection requires a MATLAB batch to be created using the SPM Batch Editor:

- Create a further directory `DIR/selection`.
- Click "Batch" in the SPM menu window (top left).
- Select "SPM >> Stats >> Bayesian Model Selection >> BMS: Maps".
- Highlight "Directory", click "Select Files" and select `DIR/selection`.
- Highlight "Data", click "New: Subject". Highlight "Subject", click "New: Session".
- Highlight "Models", click "Select Files" and select
  - `DIR/categorical/MA_cvLME_Ky_11.nii` as well as
  - `DIR/parametric/MA_cvLME_Ky_11.nii`.
- Highlight "Name models", click "New: Name" twice.
- Highlight "Name" (1st entry), click "Edit Value" and enter `GLM_cat`.
- Highlight "Name" (2nd entry), click "Edit Value" and enter `GLM_para`.
- All other options will not be used and can be left as default.
- Save this batch as `DIR/selection/design.mat`.

Once this batch has been created, model selection can be carried out as follows:

```
>> load DIR/selection/design.mat
>> MS_BMS_group_mods(matlabbatch)
```

After that, expected frequency maps (EFM) and likeliest frequency maps (LFM) for the two models have been created in the BMS directory.

(Step 3: "Group-level" selected-model maps)

Optionally, selected-model maps (SMMs) can be created as follows:

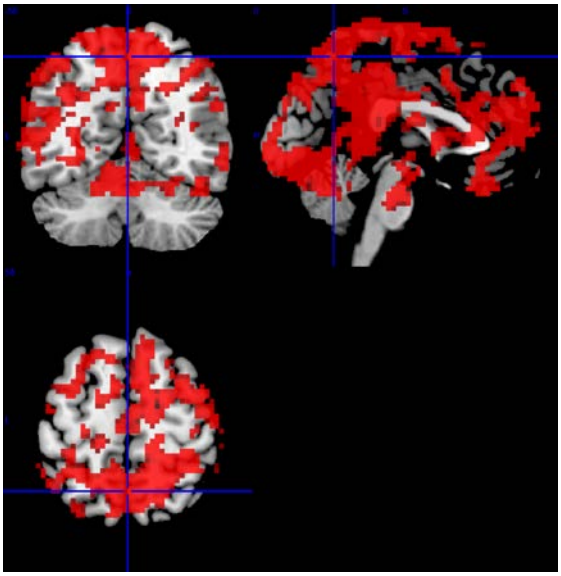
```
>> load DIR/selection/BMS.mat
>> MS_SelMod_BMS(BMS)
```

After that, SMMs for the two models have been created in the BMS sub-directory `DIR/selection/MS_SelMod_LF_10`.

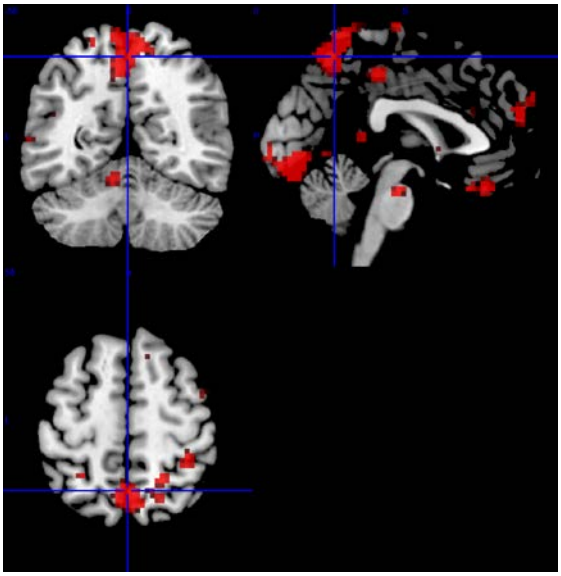
Summary: A cvBMS hands-on example

This hands-on example is summarized as "cvBMS_HandsOn.m" in the cvBMS toolkit folder.

Results: Parametric vs. categorical model



Selected-model map (SMM) for the parametric model, using an extent threshold of $k = 10$ voxels.



Likeliest frequency map (LFM) of the parametric model, thresholded at $\mathrm{LF} > 0.9999 = 99.99\ \%$.

Figure 1. *Bayesian comparison of parametric vs. categorical model.* The selected-model map (left) shows brain regions in which the parametric model outperforms the categorical model. In some of these regions (putatively parietal cortex, prefrontal cortex and insular cortex), this is due to an accuracy advantage coming from the parametric regressors. In some other regions (putatively cerebellum and white matter areas), this is due to a complexity advantage coming from the lack of HRF derivatives. The likeliest frequency map (right) illustrates brain regions with particularly strong evidence in favor of the parametric model. Although Bayesian inference on population proportions is feasible with $N = 1$, i.e. just one subject, the resulting likeliest frequencies are more closely related to subject-level posterior probabilities than to group-level frequency estimates.

Closing Remarks

Maybe or maybe not, this little toolkit will be part of a greater toolbox on Model Assessment, Comparison and Selection (MACS) in the future. Internally, this version would then be referred to as “MACS V1.0” and “MACS R2017a”.

Joram Soch, corresponding author and toolbox developer.

Carsten Allefeld & **John-Dylan Haynes**, co-authors.