Issue with basis fitting to data

Data:

TE = 35ms

Dwelltime/Bandwidth = 1200 Hz

Field Strength = 2.90 T

Basis set:

Press Siemens

TE = 35ms

Dwelltime/Bandwidth = 2500 Hz

http://juchem.bme.columbia.edu/mr-spectroscopy-basis-sets

First attempt with a 2500 Hz basis set was unsuccessful, and we received an error regarding the basis spectra covering too little time. Converted the basis to a 1200 Hz bandwidth and a 2.90 T field strength, which solved the error. However, the model fit was not good. Also attempted a 600 Hz bandwidth (half of the Hz of the original data), this produced a VERY badly fitting model. Neither of these attempts produced much concentration data, there were a lot of concentrations that read 0 or null.

MRI scanner data processed using (done in a shell script):

* Conversion of dicoms to nifti **[***spec2nii dicom -f converted\_${b} \*.dcm***]**
* Eddy correction for both water and water supressed **[***fsl\_mrs\_proc ecc --file \*d\_${p[@]}.nii.gz --reference \*w\_${p}.nii.gz --output fsl\_mrs\_proc -r --filename ecc\_metab\_${p[@]}***]**
* Centring the echo for both water and water supressed **[***fsl\_mrs\_proc truncate --file \*metab\_${t[@]}.nii.gz --points -1 --pos first --filename trunc\_metab\_${t[@]} --output fsl\_mrs\_proc2 -r***]**
* Residual water for water supressed **[***fsl\_mrs\_proc remove --file trunc\_metab\_${y[@]}.nii.gz --output fsl\_mrs\_proc3 -r --filename hlsvd\_metab\_${y[@]}***]**
* Phase correction for both water and water supressed **[***fsl\_mrs\_proc phase --file hlsvd\_metab\_${h[@]}.nii.gz --output fsl\_mrs\_proc4 -r --filename final\_metab\_${h[@]}***]**

Basis and data fitting were without error but the fit was not great.

svs\_segment -t \*${t}.nii.gz ~/spec\_analysis/converted\_${t}.nii.gz -o $homed15/\*json\_${t} -f ${t}

fsl\_mrs --data fitting/final\_metab\_${e}.nii.gz --basis ~/Basis –output fitting/fsl\_mrs\_fit\_data\_${e} --t1 T1/MR\_T1\_MPRAGE\_${e}.nii.gz --tissue\_frac json/json\_${e}/${e}\_segmentation.json --h2o fitting/final\_wref\_${e}.nii.gz --report

fsl\_mrs\_preproc command would not work – there was an error that the data had already had some pre-processing done (despite being advised that none had been done at the clinic) and so this is why each command was done separately. Specifically, the individual processing steps that didn’t work were:

- The twix commands

- DIM\_DYN and split visualisation commands

- Averaging of the water reference data

- No coil combination

- No alignment

- No data averaging

We also attempted to do processing on the basis, which created a better fit but still not perfect. This processing produced results, but some of the last steps in the processing made the fit worse despite increasing the amount of non-zero metabolite concentration values available. These were the steps used to process the basis (essentially followed the instructions on the forum):

*basis\_tools convert RawBasis\_for\_PRESSSiemens\_TE\_35\_BW\_2500\_NPts\_1024 --bandwidth 1200 --fieldstrength 2.9 basis\_1200*

*mkdir fsl\_basis\_reduced*

*cd basis\_1200*

*cp Tau.json... etc ../fsl\_basis\_reduced*

*cd ..*

*mrs\_tools vis fsl\_basis reduced*

At this point upon visualising the basis, all of the metabolites were sitting on the far left of the x-axis and not centred like in the example basis. However, we still continued processing to see how the fit would come out. The fit was slightly better at this stage.

*basis\_tools add\_set –add\_MM fsl\_basis\_reduced fsl\_basis\_with\_MM*

*cd fsl\_basis with\_MM*

*mkdir mmbits*

*mv MM\* mmbits/*

*basis\_tools conj mmbits*

At this point we produced a fitting again with the same code as earlier – the fitting was slightly better.

* Added *-- metab\_groups MM09 MM12 MM14 MM17 MM21* into the code.

This improved the fit slightly. Still not great and still getting 999 values.

* Added *-- baseline\_order -1*
* Added *-- algo MH*

After doing this all concentration values were available, however, the fit slightly worsened again.

After this we attempted to conjugate the basis again – this made no difference.

We also attempted to shift the basis (all values) by -2ppm and -1ppm.

This showed some improvements; however, it wasn’t clear how far it needed to be moved and resulted in a lot of bunching of data on the right side rather than the left.

To fix this, we attempted to scale individual metabolites to their correct locations based using the scaling feature. However, this didn’t appear to make any difference.

Lastly, we attempted to shift individual metabolites by guesswork with the shift command – this also didn’t produce any substantial improvement.

This was the best result with the basis set after most of the processing above (1200hz, baseline order, MM, algo) and the baseline itself at different phases.

Basis after initial convert function to 1200hz:



Fitting at this stage:



Basis after making reduced basis:



Basis after MM:

Fitting with just MM (data values were missing here):



Fitting with MM, flexibility, and algo (all of the concentration data was available here but the fitting was worse);



This was the fit without the algo command but with the baseline flexibility command – it appeared to give the best fit, but there were still data values missing including glutamate and GABA, both ones we needed:



This was the second best fit which was inclusive of the algo command but not the baseline command. Data was available for this one for all of the metabolites, however the fit isn’t amazing:



Shifting/scaling just produced the same sort of results with metabolites shifted to the right/left. It didn’t appear to be a good solution.