Hi Meryem.  
Here are my thoughts and results so far.  No guarantee though, please critically question all i say! :)

The oscillations/peaks in fft always occur at

**f\_o = fsample / tau**

and its higher harmonics (tau = stepsize in number of samples).

This makes sense: The regressors are weighted combinations of all (time embedded) inputs. If we repeat signals with f\_o, we will also see that periodicity within the mixed signal.

Why did I not see that before?

The reason is that you are looking into the full bandwidth of the signals that is available, which is 25Hz.   
I was so far looking only into fNIRS signals within the usual bandwidth <0.5 Hz, samples at a rate of 8.33Hz. In my analysis i used tau = 3smpl which leads to f\_o = 2.78Hz, beyond the band of interest.

What are the consequences for us?

I think we are mainly interested in investigating low frequency noise components? So this should not a problem. Depending on your band of interest, it simply means that tau should be small enough.  
For f\_o >= 25Hz, you should choose tau <= 2.   
But if for example only 10Hz and below are of interest, you can choose tau =5, etc. pp.

Mind that to increase the overall window that is considered in CCA, the number of embeddings needs to go up with shrinking tau. So we clearly have a tradeoff again, that seems quite familiar from all the FFT/windowing  rules regarding max/min observable time window and frequency band. The tradeoff is between

    1) width of frequency band of interest (higher cutoff frequency) - Stepsize

    2) width of the overall time window - Number of Embeddings and Stepsize

    3) sampling frequency

    4) total number of AUX signals used for CCA

Now for the investigation of low frequency noise components: I played around a bit and i think

tau = 2

NumOfEmb = 50

gives us all we need. A max delay of 2 seconds and a first "artifact" at 25Hz. Also a quite fine-grained embedding, which is likely a good thing. (in my previous experiments i also used a stepsize of only 3 samples, just had quite a low sampling frequency).

It is important to keep in mind, that the resulting overall window of 2s (in one direction) does only mean that only delays up to 2s between AUX and fNIRS are being observed - not that slower signals within both modalities are ignored!  
I actually do think that covering max 2s DELAY is enough.. heartbeat and respiration as well as blood-pressure changes due to movement will be covered (no way a single heart pulse will show up with 2s delay between a finger and the brain), and i can currently not think of signals that would be slower? Not saying there are none.. can you think of something that would contradict my assumption?

I did minor changes to the script, added a lowpass filter that can be turned on to possibly improve CCA performance (usually all BSS methods work better if you limit the amount of information available to that which we are actually interested in, as the unmixing focuses less on HF noise then) and both the FFT plot approaches (they seem to result in the same signals, pheew..).

So far! Let me know should you want to discuss further, also about the BCI data eventually.

Best

Alex

fsample = 50 Hz

tau [spl] = 10 6 4 2

tau [t] = 0.2 0.08 0.04

fsample / tau = 5 8.3 12.5 25

FT [h] = 5 8.3 12.5 25

FFT [l] = 5

Oscillations at fsample / tau

regardless of number of embeddings (overall time window)

looking at f < 25 Hz

f> 25 > fs / tau --> tau < fs/25 = 2