Supplementary material



Supplementary Figure 1: (a) The FC patterns used to generate the simulated data, averaged across subjects and for a "good" and "bad" example subject. (b) Time courses to simulate separated and joint expression for an example subject. (c) Final data for each subject was generated by multiplying the patterns with their associated time courses and adding Gaussian noise. (c) Estimated FC patterns with K = 4 and S = 1 or 3, spatial correlation matrix between the true FC patterns and the estimated ones, approximation error, reproducibility and stability for each of the two simulated data sets. Plots show average and standard error of each measure across folds.



Supplementary Figure 2: (a) The FC pattern used to simulate the case of a single FC topology occurring over time with varying strength. (b-c) The two estimated FC patterns represent up- and down-modulation of the same underlying FC pattern.



Supplementary Figure 3: (a) Joint expression of either 2 or 3 FC patterns results in weakly asymmetric histograms of the weights A^* . That is, an asymmetric histogram distinguishes the case of joint from separated expression. (b) Split-half reproducibility (Pearson r of least reproducible FC pattern) for data simulated with K=4 FC patterns. Errorbars represent standard deviation across splits. The drop in reproducibility is less evident for the simulation of joint expression. (c) A slightly modified measure drops below the value of 1 for K>4 for both separated and joint expression (Pearson r of least reproducible FC pattern / average absolute value of Pearson r of non-matched FC pattern pairs). (d) This modified measure would also work for the case K=3. (e) The skewness of the weights A^* again distinguishes joint from separated expression. The skewness of the weights for 4 task-based FC patterns, lies in between the two cases.



Supplementary Figure 4: Weights **A*** of FC pattern 4 arranged by window x (task x subject). Strong correlations during the music task exist for most subjects, indicating that this FC pattern is not specific to individual subjects.



Supplementary Figure 5: Comparison of FC patterns estimated using k-means clustering, k-SVD (S=1, S=3) and truncated SVD to represent task-based dFC. S=1 generalizes k-means and has flexible weights, and S=3 generalizes PCA and imposes no orthogonality. For k-SVD we obtained better results for K=2 because of the anti-correlation between the average dFC of the subtraction task and the other two tasks, and because negative weights allow the sign of the FC pattern to flip. That is, for K=2 and S=1 the first FC pattern correlated with a flipped version of average memory dFC (r=-0.75), and for S=2 it correlated with a flipped version of average memory dFC (r=-0.77). In contrast, for K=3 the minimal Pearson r was 0.65 and 0.54 for S=1 and S=3, respectively. For PCA, the number next to the FC pattern indicates its rank, which relates to their relative importance in terms of explained variance. Correlation matrices show Pearson r with average dFC during each task (r value indicated if >0.4).



Supplementary Figure 6: Comparison of K=3 FC patterns estimated using k-means clustering, k-SVD (S=1, S=3) and truncated SVD to approximate resting-state dFC. S=1 generalizes k-means as it has flexible weights, S=3 generalizes PCA as it imposes no orthogonality. For k-SVD we again used K=2 only because of the anti-correlation between the first two FC patterns (see also the legend of Supplementary Fig. 5). For truncated SVD, the number next to the FC pattern indicates its rank, which relates to their relative importance in terms of explained variance. Correlation matrices show Pearson r with FC patterns estimated using k-means clustering (r value indicated if >0.4).