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Non-Negative Decomposition of Structural Connectivity in the Developing Brain

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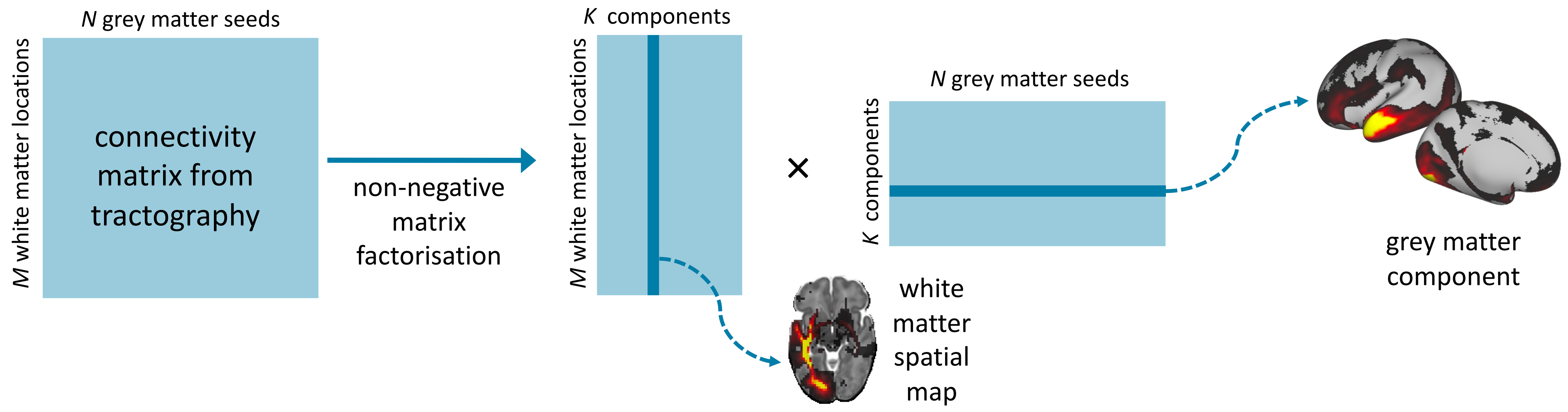
Introduction

During the neonatal period, the brain grows and develops rapidly, which can make it challenging to ensure correspondence between templates at different time points. Previously, we presented a data-driven framework to map white matter bundles and their corresponding grey matter termination points from neonatal dMRI data, without the need for pre-defined regions of interest [1]. Here, we validate our non-negative method using simulated data, and extend the framework to generate cortical parcellation schemes. We also develop a method for non-negative dual regression to obtain subject-specific connectivity maps.

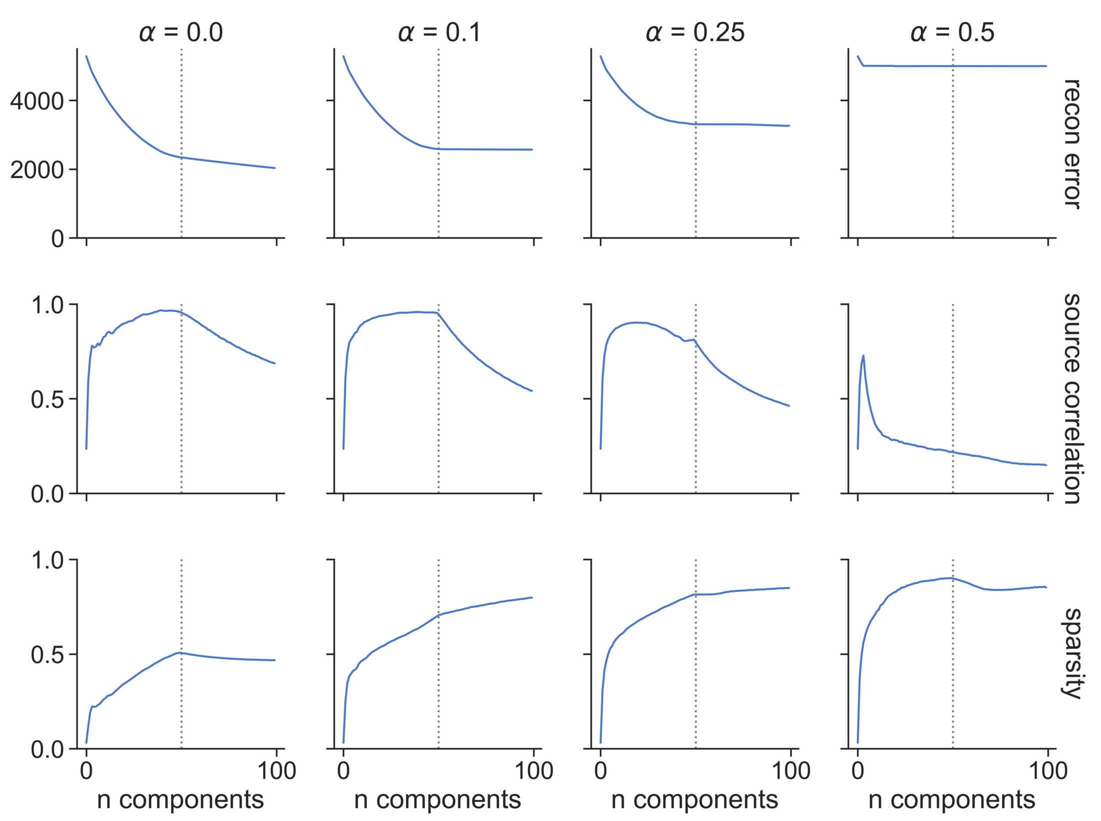
Methods



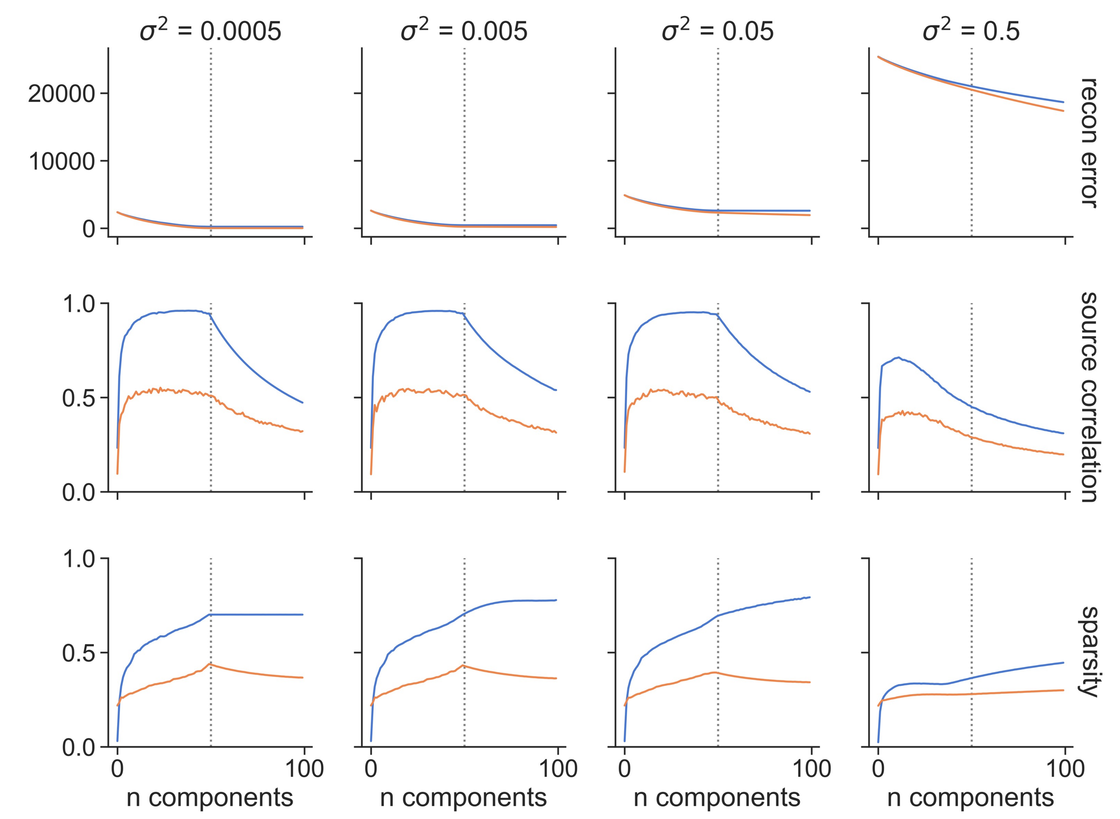
Using MRI data from 323 term-age subjects from the developing Human Connectome Project [2,3], we performed probabilistic tractography to generate grey-matter to whole brain connectivity matrices. Applying non-negative matrix factorization (NMF) [4] to the group-averaged matrix yields a set of grey matter components and their corresponding white matter connections.

Simulations

We tested the framework on simulated data to observe the results on a system where we know the ground truth. Sources **S** were modelled as log-beta distributions, based on real data. The simulated data were calculated as **X** = **AS**, and Gaussian noise was applied to the data via a logit transform, to maintain non-negativity. We compared the performance of NMF with ICA, another matrix decomposition technique that had been used in this context [5], looking at the effect of altering the regularization parameter, α, and increasing the variance of the noise, σ^2.



Increasing α increases sparsity, but also increases the reconstruction error. The NMF decomposition breaks down for high regularisation. α = 0.1 is a good middle ground, balancing reconstruction accuracy and sparsity.



Reconstruction error = $\Sigma(\mathbf{X} - \mathbf{AS})^2$, information lost through the decomposition

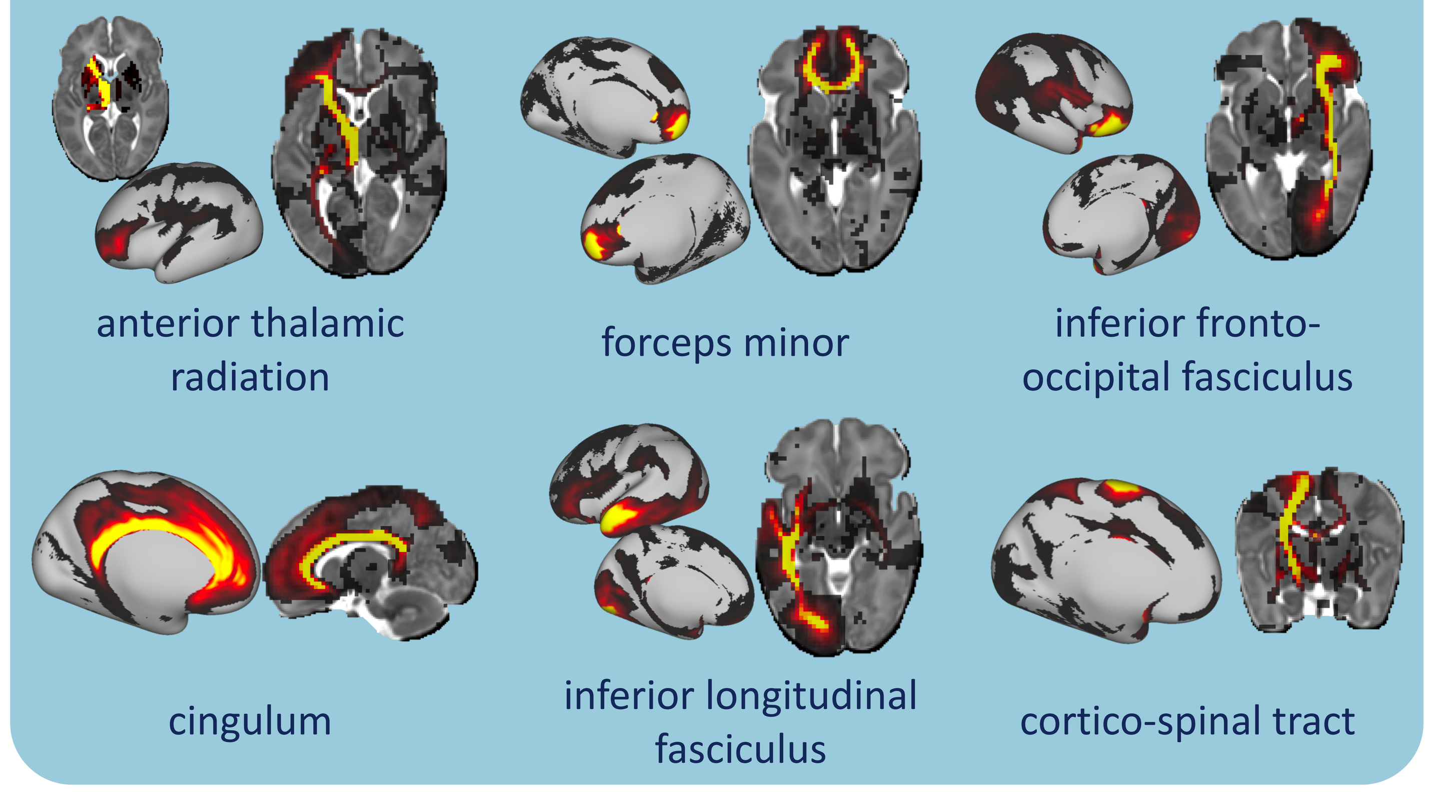
The average correlation value between best-matched sources and components

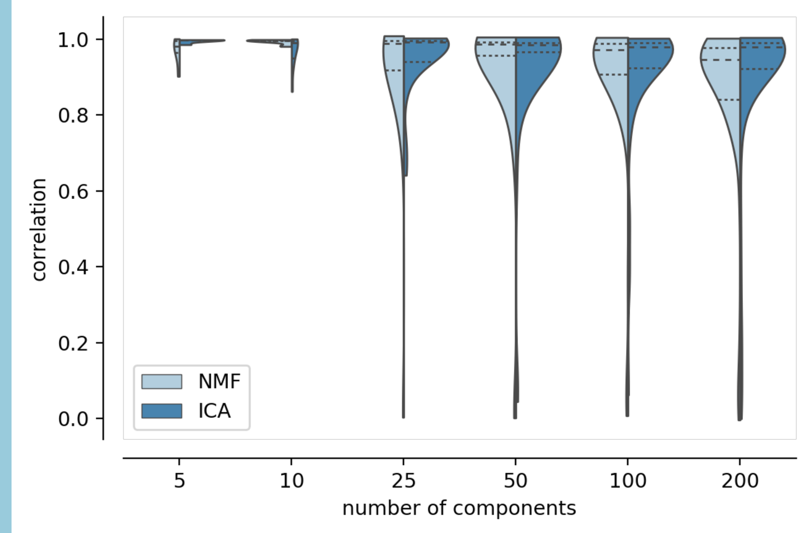
Sparsity of the derived components

Reconstruction error increases with noise, whereas source correlation and component sparsity decrease. The decompositions are robust to the levels of noise we would expect in real data (σ^2 = 0.05). NMF components correlate more strongly with the true signals, and are more sparse than ICA components.

In-vivo Results

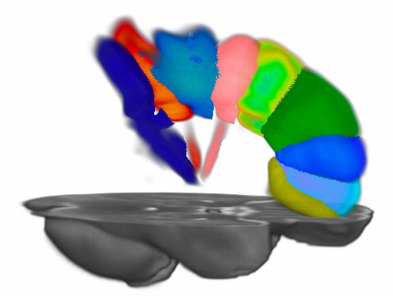
Components correspond to white matter tracts:





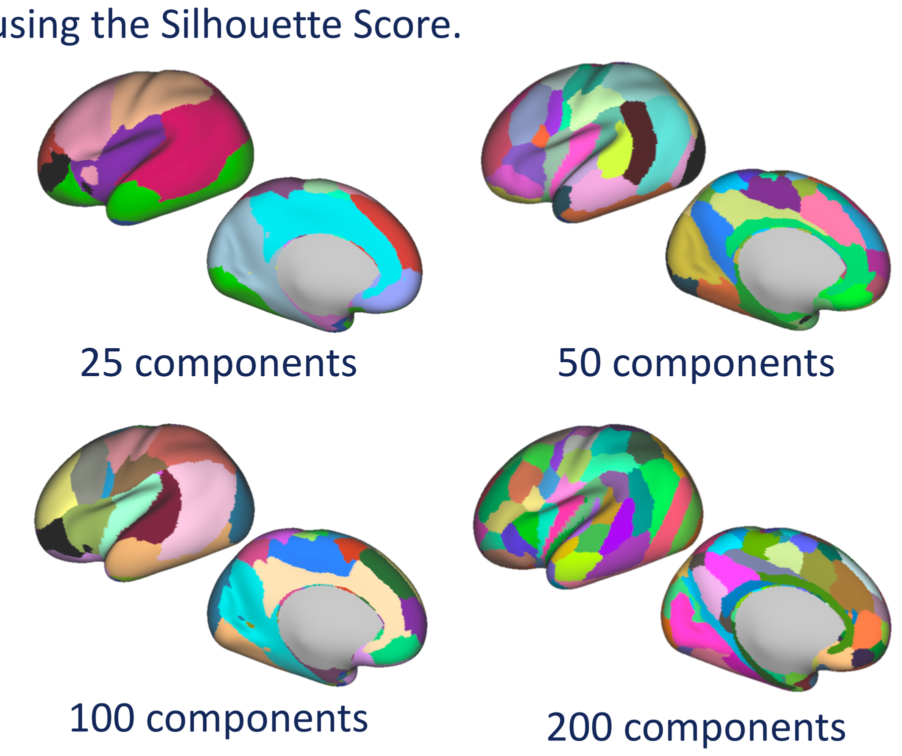
NMF components are robust in a split-half analysis of the cohort. Correlation scores across the split-half are similar to ICA.

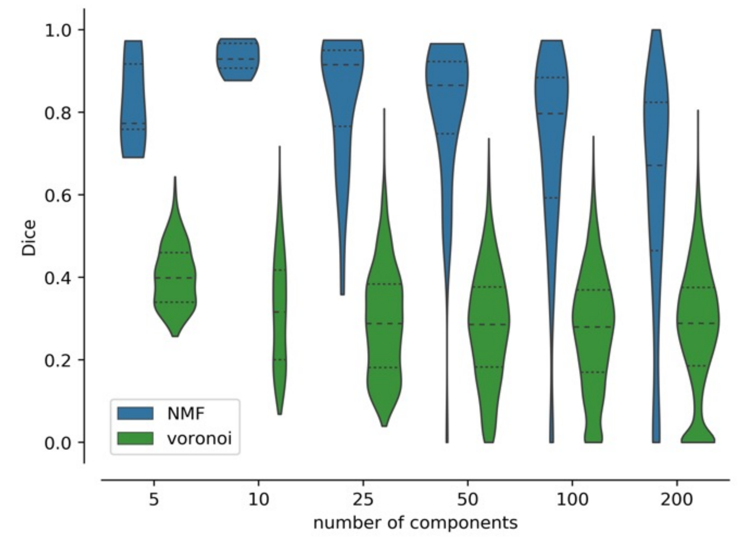
White matter components provide a data-driven segmentation of the corpus callosum



Parcellations

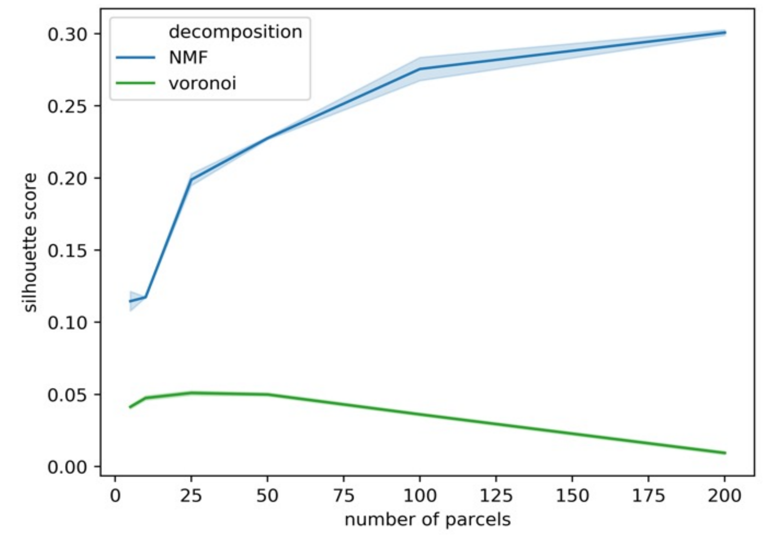
Grey matter components were used to parcellate the cortex, using a "winner-takes-all" approach. We performed parcellations for each half of the cohort, and measured the spatial overlap using Dice scores. We also assessed how well the parcellation clusters similarly connected vertices using the Silhouette Score.





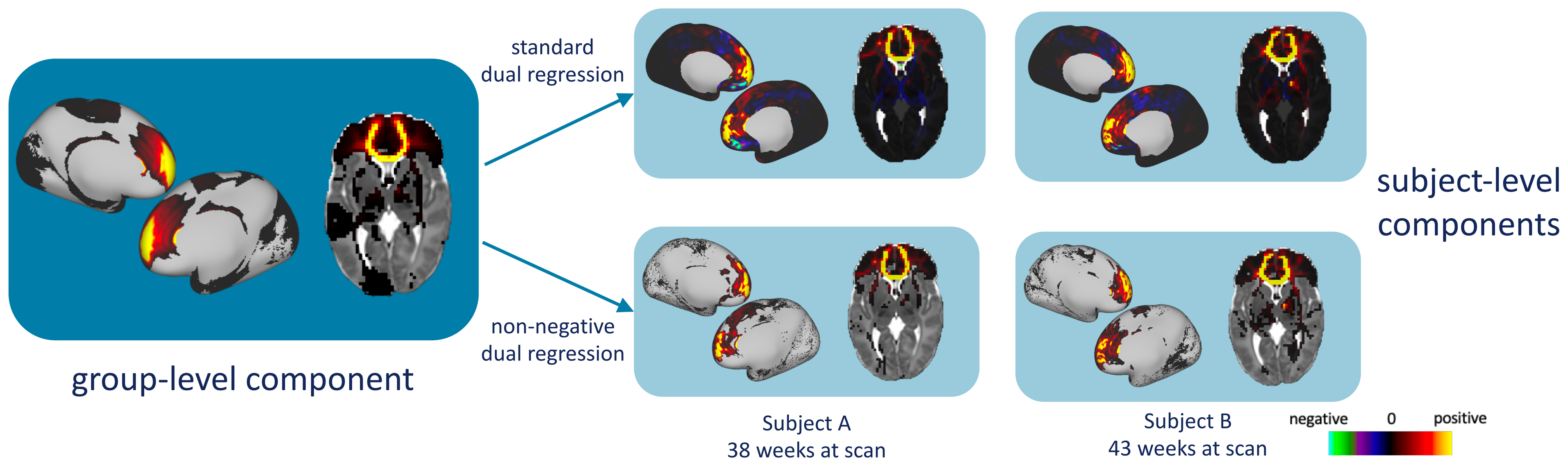
Parcellations across the split-half were more similar than random Voronoi parcellations

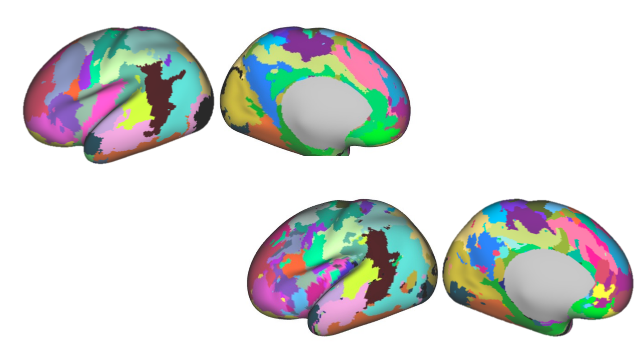
The data-driven parcellation effectively groups similar vertices



Non-Negative Dual Regression

Dual regression can be used to generate subject-level representations of group components and mixing matrices [6]. The standard approach involves taking the pseudoinverse of the connectivity matrix, which introduces negative values into the components and their weights. Instead, we have developed a "non-negative dual regression" technique for back projecting NMF results, using non-negative least squares (NNLS).





Dual regressed grey matter components can be used to generate subject specific parcellations

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References: **[1]** Thompson et al, OHBM (2019). **[2]** Hughes et al, Magnetic Resonance in Medicine (2017). **[3]** Bastiani et al. Neuroimage (2018). **[4]** Lee & Seung, Advances in Neural Information Processing Systems (2001). **[5]** O'Muircheartaigh and Jbabdi, Neuroimage (2017). **[6]** Beckmann et al, Neuroimage (2009).