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Characterization of Cognitive Structure Using Explainable Models and Multimodal Neuroimaging Maps

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Understanding the emergence of cognitive operations from the brain's topographical organization is a fundamental goal in neuroscience. However, the roles and interactions of functional, structural and chemical brain features in shaping cognitive structure have remained poorly characterized. This study aims to investigate these multimodal contributions to cognitive structure from a spatial patterning perspective.

We used a comprehensive set of 48 brain maps from Neuromaps, encompassing functional MRI, structural MRI, PET and ASL. The data were collected from independent laboratories. To assess cognitive structure, we focused on CogPC1, a derivative component from Neurosynth, which represents the primary axis of variance in functional cognition. To examine the relationships between brain multimodal features and CogPC1, we conducted two analyses. First, we created a correlation matrix to identify and rank brain features, capturing linear associations. Second, we developed machine learning models to predict CogPC1 to explore more complex patterns, including non-linear relationships and interactions among brain features. We created a general model using all modalities, along with four additional models, each based on a single modality. To ensure robust results in each model, we applied a five-fold cross-validation approach, and for explainability in the model, we calculated the Shapley additive explanations, a technique that utilizes game theory to determine the contribution of each variable to individual model output.

The correlation analysis of the brain maps revealed a strong negative correlation between CogPC1 and Functional Connectivity (FC) gradient 1 (r= -0.66), followed by a positive correlation with the norepinephrine transporter (r= 0.50) (Fig.1). Additionally, there was a negative correlation with sensory association areas (r= -0.49) and another negative correlation with FC gradient 7 (r= -0.36) (Fig.1). Among the three structural maps, the evolutionary cortical expansion map showed the highest correlation (r= -0.24) (Fig.1). For the ML models, the general model outperforms unimodal models, explaining over 80% of the variance in CogPC1 (Fig. 2a). In the general model, we found that functional connectivity in gradients 1, 7, and 6 had the highest contributions to predicting CogPC1, all exerting negative influences (Fig. 2b). Among the neurotransmitter modalities, the norepinephrine transporter was the top contributor, showing a positive influence on CogPC1. A clear interaction effect with gradient 1 is visible on gradients 7 and 6 and norepinephrine transporter (Fig. 2c-f). The contribution of these features to CogPC1 varies according to the gradient 1 spectrum, affecting the slope, direction and magnitude of their relationship with CogPC1.

Our results reveal that functional connectivity gradients and neurotransmitter density maps of receptors and transporters are key predictors of cognitive structure. Gradient 1, in particular, plays a crucial role in interacting with other brain features, suggesting that it encodes the operational regime of other brain features. This study highlights the importance of multimodal integration in understanding cognitive structure and provides insights into the complex interactions between different brain features. These insights could pave the way for personalized medicine, offering more precise brain-based assessments and individualized treatments for cognitive and neurological disorders.

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