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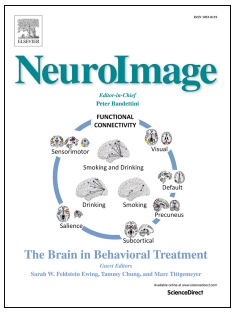

Bayesian Optimisation of Large-Scale Biophysical Networks

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Bayesian Optimisation of Large-Scale Biophysical Networks

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Abstract

The relationship between structure and function in the human brain is well established, but not yet well characterised. Large-scale biophysical models allow us to investigate this relationship, by leveraging structural information (*e.g.* derived from diffusion tractography) in order to couple dynamical models of local neuronal activity into networks of interacting regions distributed across the cortex. In practice however, these models are difficult to parametrise, and their simulation is often delicate and computationally expensive. This undermines the experimental aspect of scientific modelling, and stands in the way of comparing different parametrisations, network architectures, or models in general, with confidence. Here, we advocate the use of Bayesian optimisation for assessing the capabilities of biophysical network models, given a set of desired properties (*e.g.* band-specific functional connectivity); and in turn the use of this assessment as a principled basis for incremental modelling and model comparison. We adapt an optimisation method designed to cope with costly, high-dimensional, non-convex problems, and demonstrate its use and effectiveness. Using five parameters controlling key aspects of our model, we find that this method is able to converge to regions of high functional similarity with real MEG data, with very few samples given the number of parameters, without getting stuck in local extrema, and while building and exploiting a map of uncertainty defined smoothly across the parameter space. We compare the results obtained using different methods of structural connectivity estimation from diffusion tractography, and find that one method leads to better simulations.

Keywords: biophysical model, simulation, Bayesian optimisation, resting-state, diffusion, MEG

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