Brain Modeling Project: Classifying Brain States Using The Virtual Brain and Machine Learning

Doga Tekeli 513237

May 22, 2025

Abstract

This project simulates brain dynamics using The Virtual Brain (TVB) framework to differentiate between resting and stimulated brain states. A set of simulations were performed across multiple brain regions using a generic 2D oscillator model that we saw during the labs. Statistical features were extracted from the resulting neural activity and used as input for machine learning classifiers.

Goals

The main objective of this project is to evaluate whether large-scale brain simulations generated by The Virtual Brain (TVB) can be used to classify different brain states. Specifically, we aim to distinguish between resting-state dynamics and states influenced by external stimulation using classical machine learning models.

Methods

1. TVB Simulation

The simulations were performed using The Virtual Brain (TVB) framework. I used the default structural connectivity matrix provided by TVB, consisting 76 cortical and subcortical brain regions. The connectivity matrix includes both region-wise weights and tract lengths, derived from diffusion tensor imaging. Each brain region was modeled using the **Generic 2D Oscillator** neural mass model that we have seen during the labs, which captures basic excitatory-inhibitory dynamics through two coupled differential equations:

$$\dot{V} = d\,\tau\left(-fV^3 + eV^2 + gV + \alpha W + \gamma I\right)$$
$$\dot{W} = \frac{d}{\tau}\left(cV^2 + bV - \beta W + a\right)$$

[2]

Here, V and W represent the fast and slow neural variables, respectively. The parameters a, b, c, d, e, f, g, α, β, γ, τ control the oscillator's dynamics, and I corresponds to external input. For better predictions of the Machine Learning part of my project, variability across simulations is added with the parameter c being randomly sampled from the interval $[0.4, 0.6]$.

Simulations were run for 1000 ms (1 second) under two conditions: Resting State with no external stimulation applied and Stimulated State where a pulse-train stimulus was applied to a randomly selected posterior brain region (regions 45–53). The stimulation was modeled as a temporal pulse train with an onset at 200 ms, duration $T = 500$ ms, and decay constant $\tau = 50$ ms. For each simulation, the neural activity time series of all regions were summarized by computing the mean, variance, and peak-to-peak amplitude, resulting in a feature vector of length $3 \times 76 = 228$ per sample. [3] [1]

2. Machine Learning

We created a dataset of 200 simulations (100 resting, 100 stimulated) using features extracted from large-scale TVB simulations. Multiple classifiers were evaluated using 5-fold cross-validation: Logistic Regression, Support Vector Machine, Random Forest, Decision Tree, Gaussian Naive Bayes, and K-Nearest Neighbors. A train-test split (70/30) was used to evaluate final performance, with a focus on F1-score and ROC curves.

Results

We found that Logistic Regression classifier gives the best result in distinguishing between resting-state and stimulus-evoked brain activity. The classifier achieved an **accuracy of 77%** on the test set. While the model performed strongly in identifying resting-state samples (high recall), it was comparatively less effective at detecting stimulus-evoked samples, as reflected in the lower recall for class 1 (stimulus).

The overall **macro-averaged F1-score was 0.76**, indicating a balanced performance across both classes. The ROC curve at the end of the project demonstrates that the classifier is good at distinguishing the classes, with an **Area Under the Curve (AUC) of 0.87**, suggesting good separability between the two states. Future work could focus on improving the recall for stimulus detection by exploring more complex models or using a bigger dataset.

References

[1] Maria Laura Degrazia. The virtual brain lab 1, 2025. https://colab.research.google.com/drive/1oAjnXhCULta8HPjO5B-ge3r71ZAnW2iT.html.

[2] The Virtual Brain Project. Generic 2d oscillator, 2024. https://docs.thevirtualbrain.org/_modules/tvb/simulator/models/oscillator.html.

[3] The Virtual Brain Project. The virtual brain documentation, 2024. https://docs.thevirtualbrain.org/py-modindex.html.