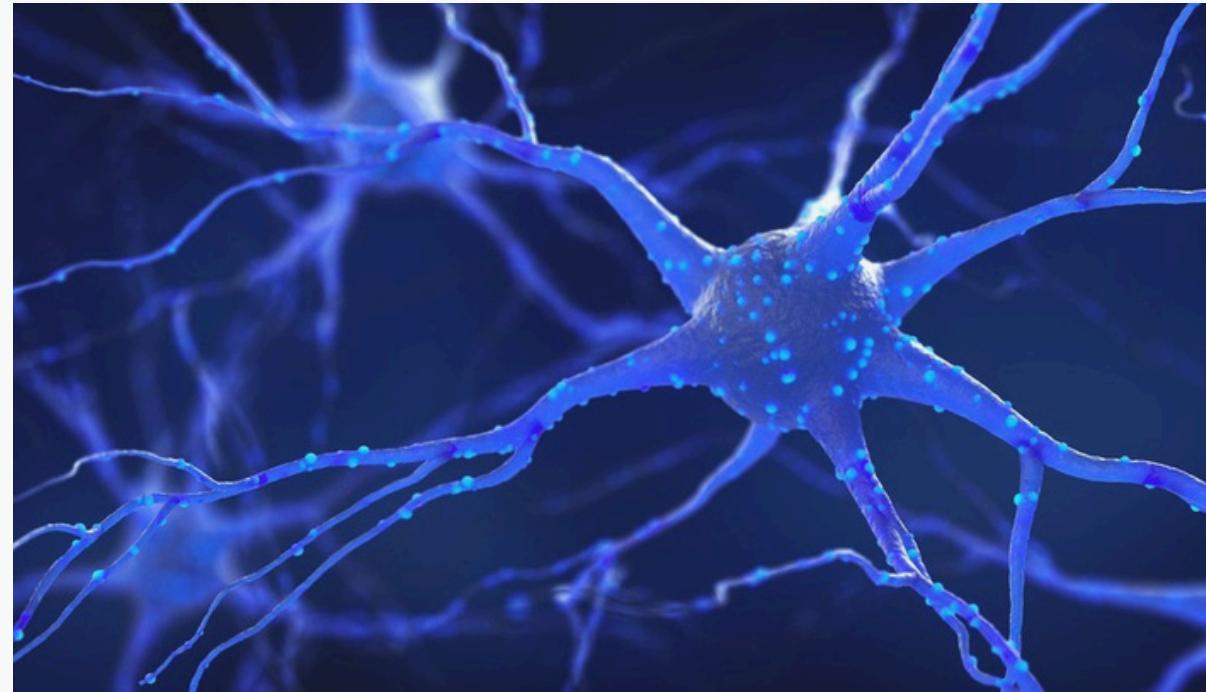




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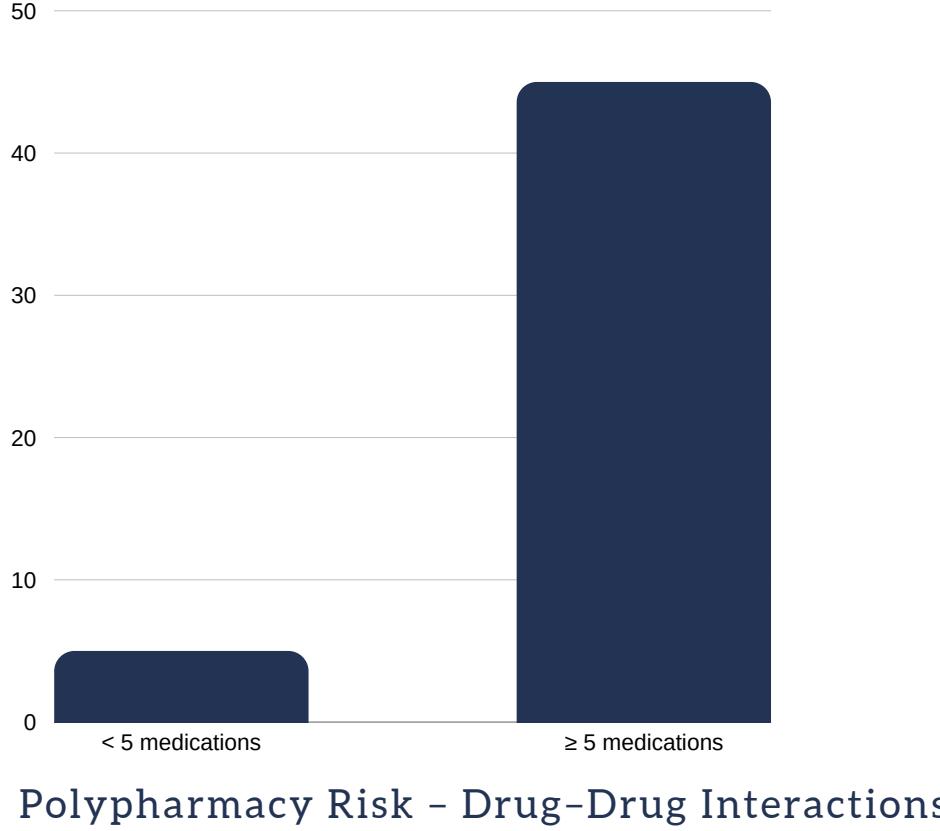
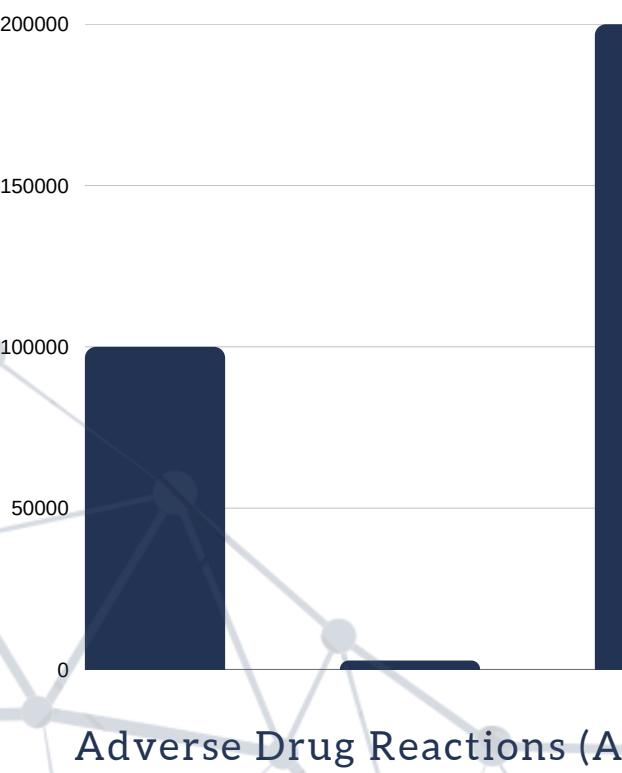
VIRTUAL NEURON CLONING AND DRUG SIMULATION

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PROBLEM & MOTIVATION:

The Issue Conventional drug testing for neuroscience is:

- Expensive
- Morally challenging
- Individual differences in neurons are significant, based on population-level assumptions.
- Drug testing must be scalable, safe, and personalized.



Adverse reactions to prescribed medications are a growing concern worldwide, with neurological drugs often involved. As the number of affected patients increases, there is a clear need for safer and more precise methods to predict individual drug responses.

PROJECT OVERVIEW:

We have developed a platform that uses artificial intelligence (AI) to digitally replicate any biological neuron using real electrophysiological data, such as voltage, current, and time. Our system learns the underlying dynamics of the original neuron from data and creates a digital twin that performs similarly by using a data-driven deep learning pipeline (CNN + LSTM) to predict neuron parameters from V and I. This enables us to simulate the way that drugs affect neurons.

PROJECT OBJECTIVES:

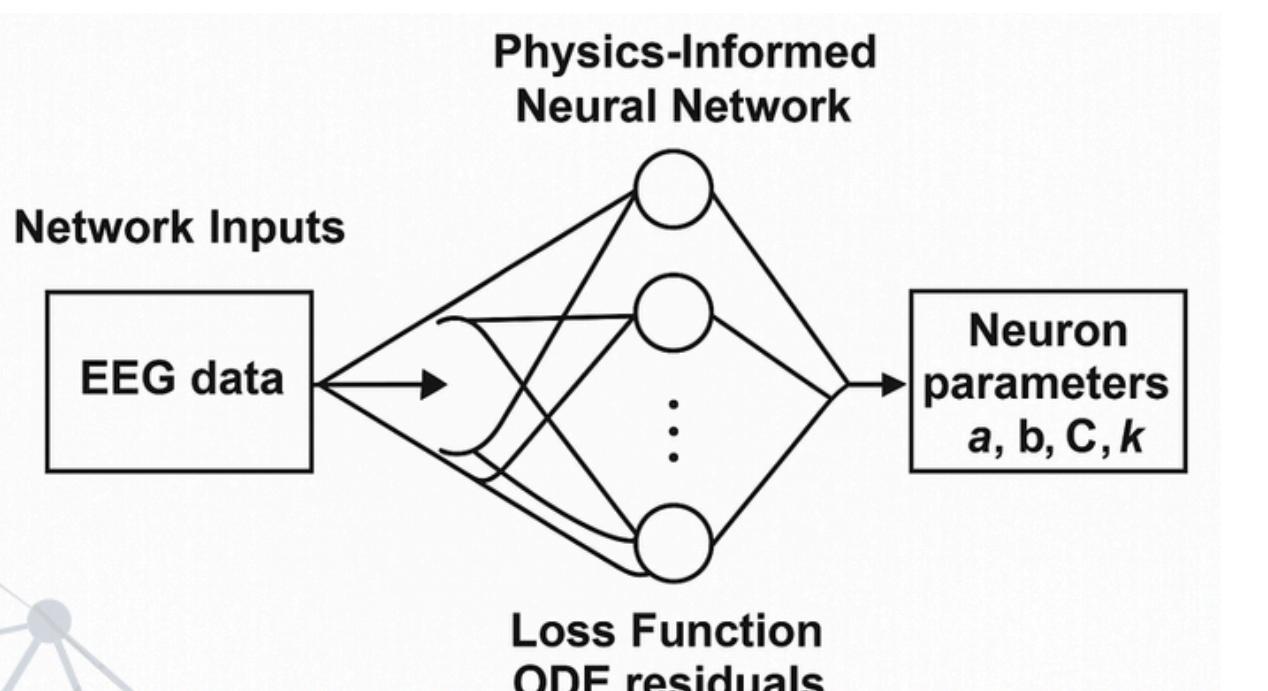
Key Goals The electrical signature of any neuron can be used to create a clone. Simulate how neurons respond to different stimuli or circumstances. Make predictions about the effects of medications without actually giving them. Provide a system for comprehensive, customized online drug testing.



OUR RESOLUTION ,OUR METHOD

We create individualized, biologically accurate neuron models by fusing AI and neuroscience:

- Fast solvers and constrained parameters are used to simulate a variety of neurons.
- Infer neuron characteristics from voltage and current signals using a CNN+LSTM model.
- Learn how drugs change the dynamics of the brain to model their effects.
- Facilitate virtual treatment testing and quick, equation-free prediction.



A Block Flow Diagram summarizes the overall process flow in a simplified and organized manner.

HOW IT OPERATES:

Step 1 :

Neuron Cloning - From Simulations to Deep Learning

Goal: Create a digital twin of a real biological neuron using deep learning pipeline trained on simulated neuron data.

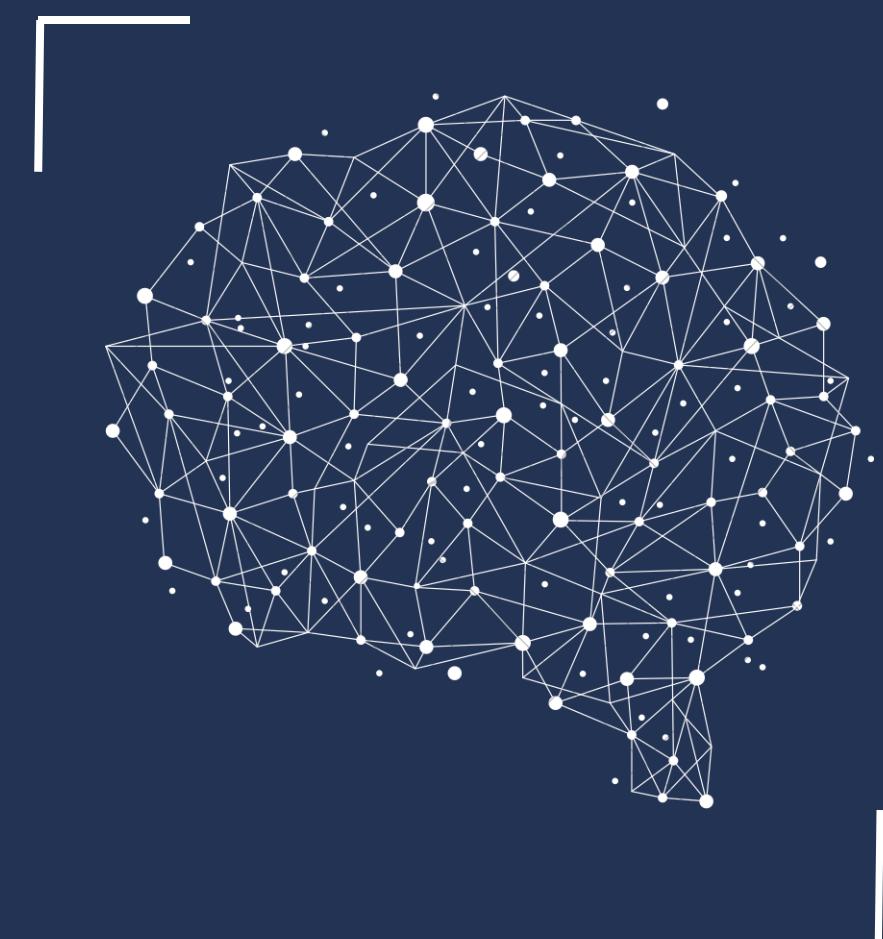
Time-series electrophysiological data as inputs:

Voltage: $V(t)$, the membrane potential over time

Current: Time-varying input stimulus, $I(t)$

Time: vector of time, t

These signals, which are obtained from patch-clamp recordings or comparable electrophysiological tests, can be fed into a CNN + LSTM model that has been trained to predict the internal parameters of the neuron.



Neuron Cloning - From
Simulations to Deep Learning

Method:

To create time-series data, we use biophysically realistic models (like Hodgkin-Huxley) to simulate various neurons and solve them numerically (like the Explicit Euler method).

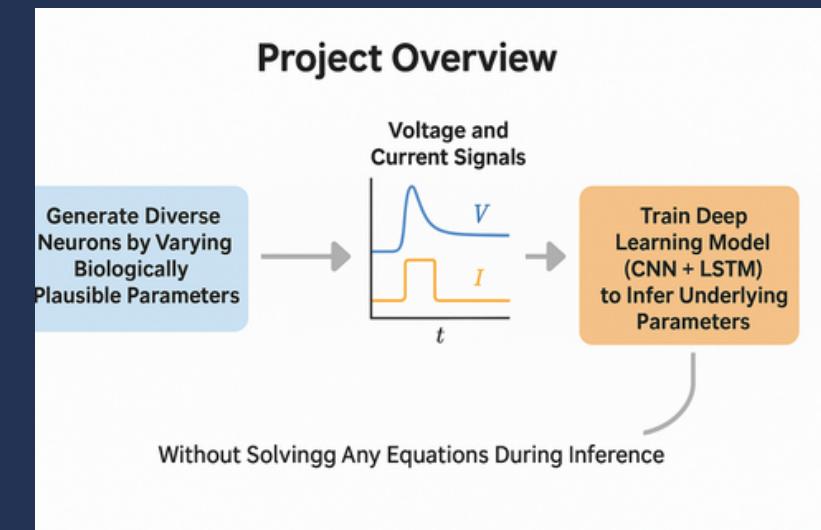
The inverse mapping is then taught to a deep learning model (CNN + LSTM):

From: Signals for voltage ($V(t)$) and current ($I(t)$)

To: Fundamental neuronal characteristics like membrane capacitance (C)

Conductances of ions (g_{Na} , g_K , etc.)

Activation/inactivation gating dynamics



Simulate neuron activity and use deep learning to recover its parameters instantly.

Benefit:

Quick, equation-free deduction Differential equations do not need to be solved at runtime.
readily expands to big datasets or real-time applications
keeps biophysical plausibility by using simulations based on physics for training.

Results:

The neuron's high-fidelity digital twin:
Realistic electrophysiology
Set up and prepared for subsequent tasks such as customized neural modeling or drug simulation



Step 2 :

Drug Effect Learning

Goal: Learn how different drugs alter neural behavior by modeling their effects on the neuron's underlying biophysical parameters.

Data Gathering:

Prior to and following drug administration, record electrophysiological signals, noting characteristics like:

Input currents ($I(t)$) and voltage traces ($V(t)$)

Rates of firing

Shape, amplitude, and width of an action potential

Refractory periods, latency, and spiking threshold

A subsequent model uses these paired recordings as input and learns to:

Identify signal alterations brought on by particular medications.

Estimate how the drug's action will change the underlying neuron parameters.

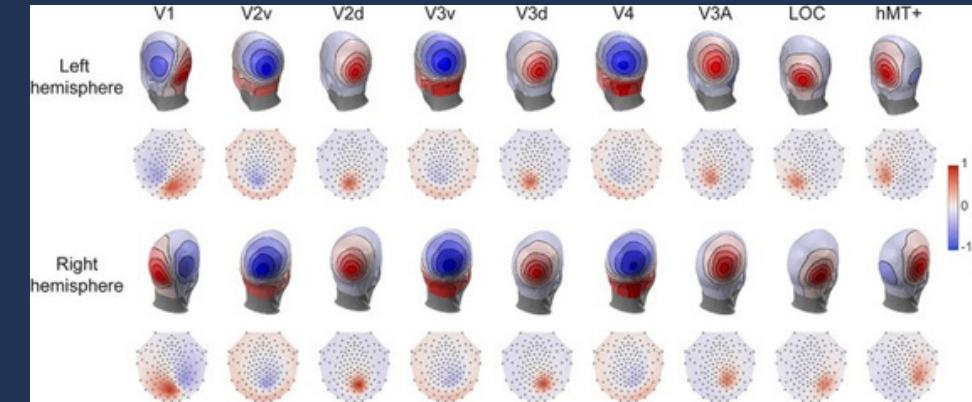
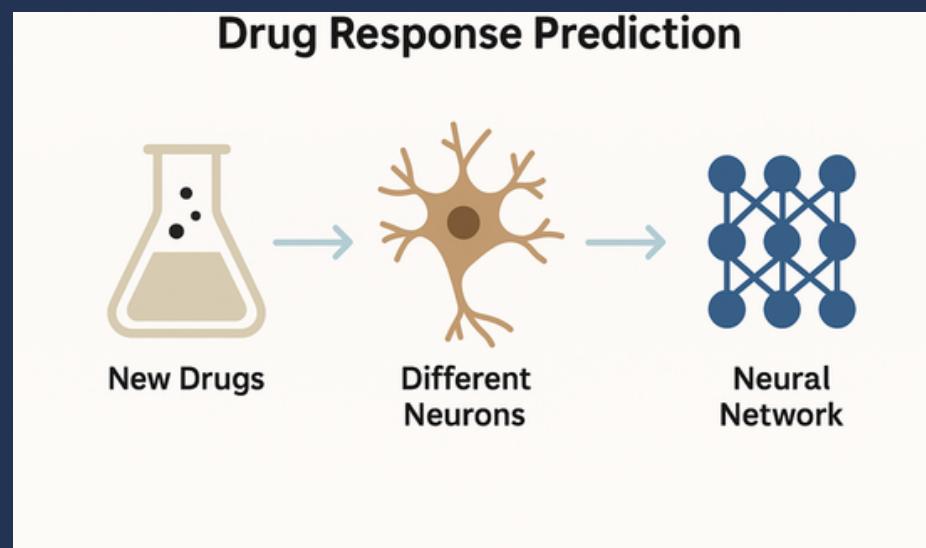


Figure Representative EEG trace illustrating brain electrical activity recorded from scalp electrodes.



Predict how a drug changes neuro behavior using signal-based neural models.

Second Model Training:

To detect parameter shifts brought on by drugs (such as sodium channel blockage resulting in decreased $g_{Na} \cdot g_Na$), a drug effect model is trained.

Find out how the behavior of the neuron is altered by each type of medication.

Mechanism:

Functions similarly to a differential analyzer

$$\Delta \text{Parameter} = f(\text{Drug Type}, \text{Dose})$$

Use: Current digital neuron clones can now have their drug effects predicted.

Even from patients who aren't visible, new neurons can be created using just their baseline data.

Step 3: In-Silico Drug Testing

Goal: Rapidly simulate how a neuron will respond to a drug without using physical experiments.

Pipeline Integration:

Use the CNN + LSTM model (from Step 1) to clone the neuron.

Use the drug-induced signal or parameter changes you learned (from Step 2).

Use quick numerical solvers to model the altered neuron response.

Result:

According to the model, the neuron will:

- Burns (or doesn't burn)
- Changes in the threshold, amplitude, or frequency of spikes
- Depending on the drug type and dosage, it becomes excited, inhibited, or silenced.

Examples of Use:

- Determine whether a drug:
- will soothe agitated neurons (e.g., epilepsy)
- could cause adverse effects by over-inhibiting
- is responsive or ineffective for the patient's profile

Benefits:

- Fast (minutes rather than days)
- Safe (no biological damage)
- Customized (able to adjust to neuron clones unique to each patient)

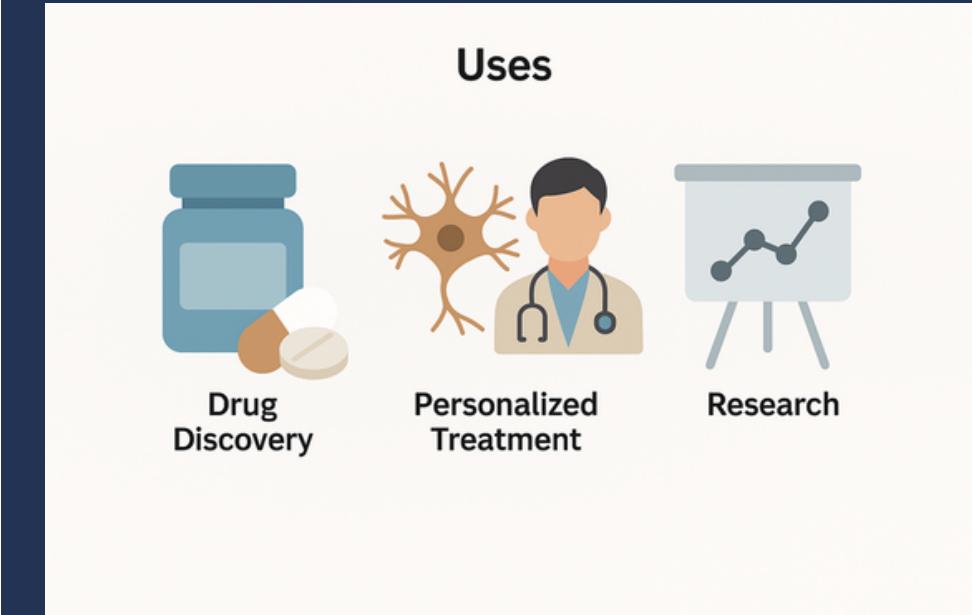
USES - PRACTICAL APPLICATIONS OF THE MODEL

1. Customized Neuropharmacology

- Model the neuron's reaction to medication in a particular patient.
- Customize therapies for conditions like Parkinson's, depression, and epilepsy.
- Minimize adverse effects and prescription trial-and-error

2. Pharmaceutical R&D

- Use virtual neurons to test thousands of compounds.
- Early drug structure optimization and neurotoxicity detection are important.
- lowers development costs and speeds up discovery.



Enables drug testing,
personalized treatment, and
ethical neuroscience research.

3. Medical Education

- Interactive, three-dimensional neuron models for training students.
- visualization of drug effects and spikes in real time.
- An ethical, reusable, and safe teaching option.

4. Ethical Research & Regulation

- reduces the need for testing on humans and animals.
- supports the three Rs: Refine, Reduce, Replace.
- helps adhere to REACH, FDA, and EMA ethical standards.

PRELIMINARY RESULTS FIRST DISCOVERIES :

- Our CNN + LSTM model trained on simulated data can accurately reconstruct the dynamics of neurons.
- Real voltage and current signals are successfully used by the model to infer parameters that are biologically plausible.
- Increased inhibition, for example, is consistent with anticipated physiological reactions in drug simulations.
- Experimental (real-world) recordings are being used for validation, and the results show encouraging consistency.

INITIAL FINDINGS WITH CNN + LSTM

1. Behavior of Neurons Similar to Hodgkin-Huxley models, reconstructed PINNs were able to accurately learn neuron dynamics (like thresholds and spiking) from sparse data.
2. Complementary Biology with Drug Simulations
The way that simulated reactions to GABA and glutamate medications match observed effects is proof that the model accurately represents neurophysiology.
3. There is ongoing experimental validation.
When comparing early tests with lab data, the accuracy of drug response and spike prediction is high.
The primary objective is to improve performance in noisy, real-world datasets.

RESULTS - MODEL EVALUATION:

With a robust R2 score of 0.73 and an overall MSE of 184.2, our model demonstrated good overall accuracy.

Performance by parameter:

Outstanding forecasts were made for:

R2 – C (membrane capacitance) = 0.87

Resting Potential (vr) – R2 = 0.96

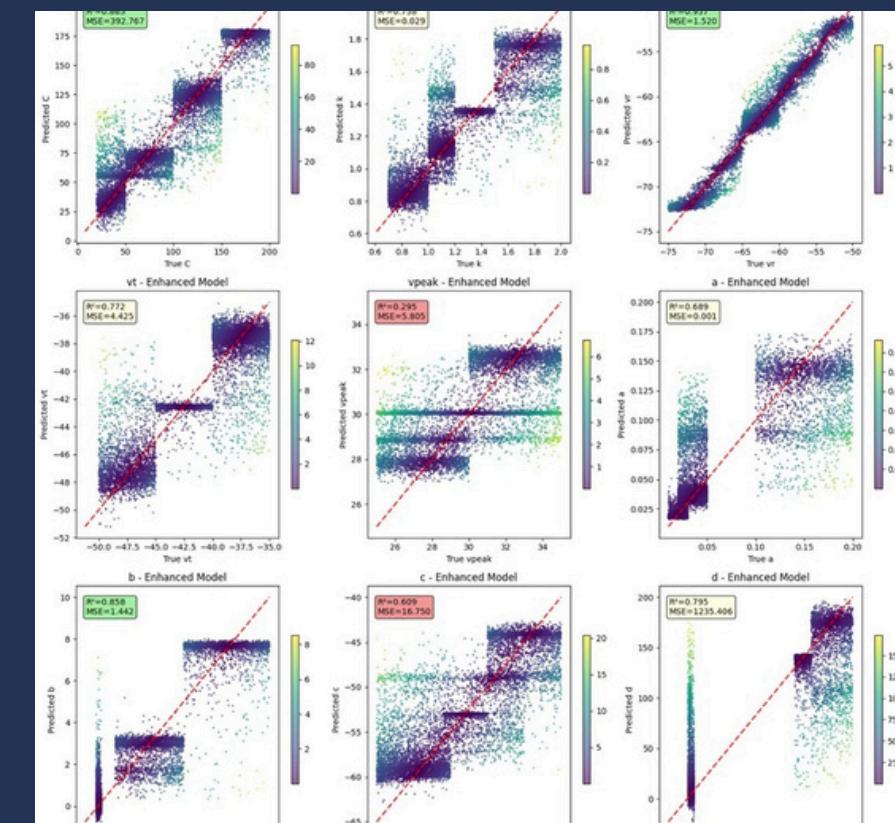
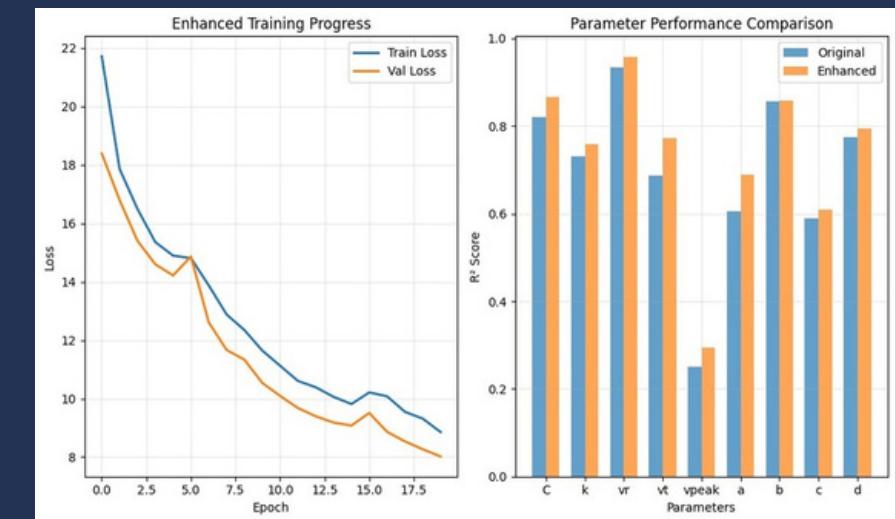
R2 = 0.86 – b (Recovery Sensitivity)

There were positive forecasts for:

R2 scores for k, vt, a, and d range from 0.69 to 0.79.

Improvement is required:

Spike Peak Voltage (vpeak) – R2 = 0.29



CONCLUSION :

FROM NETWORKS TO PERSONALIZED NEUROSCIENCE:

By modeling realistic neural networks to investigate communication, drug effects, and seizure-like behavior, we hope to transform neuroscience.

We customize neuron models for more precise and moral drug testing by incorporating patient data (EMG, prescriptions, EMRs).

Our goal is to safely and individually predict drug responses, beginning with virtual neurons prior to actual trials.

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THE INTERSECTION OF SCIENCE AND EMPATHY
FOR SAFER, MORE INTELLIGENT NEUROSCIENCE

THANK YOU