Physics-Informed Neural Networks to Predict Drug Absorption Kinetics

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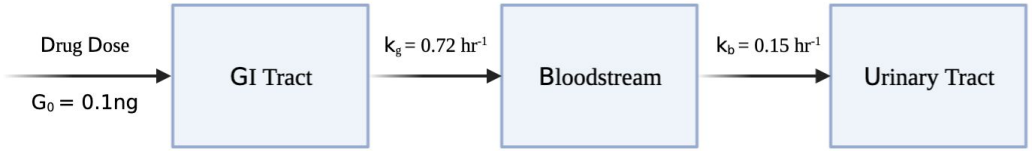
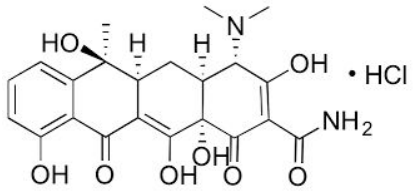
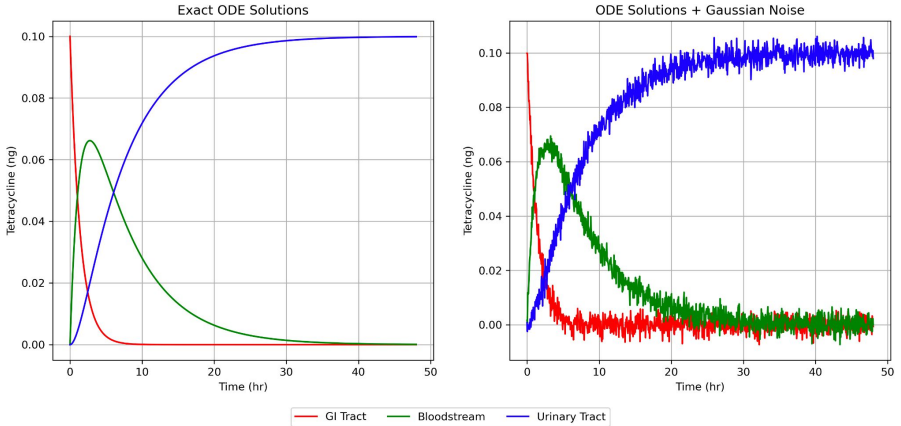
Background



Goal: design PINN to model human pharmacokinetics of broad-spectrum antibiotic tetracycline HCl



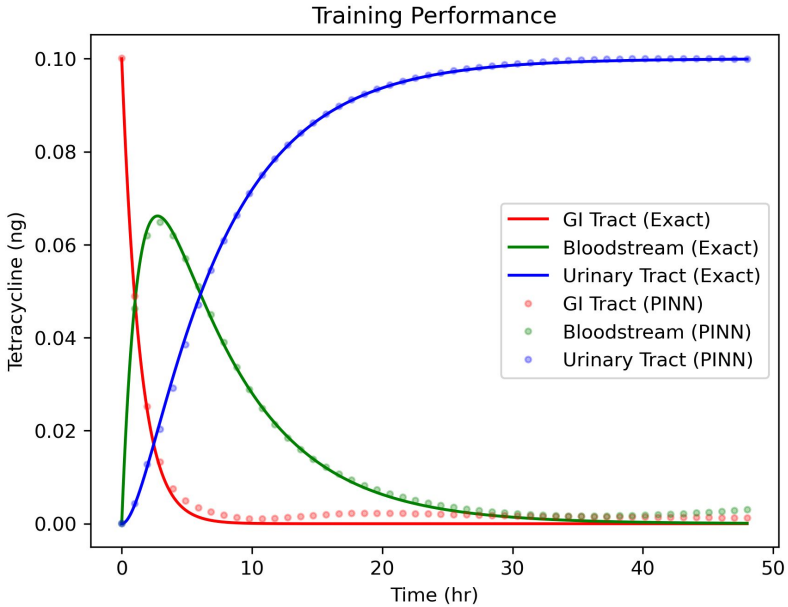
$$\frac{dB}{dt} = k_g G - k_b B, \quad B(0) = 0$$
$$\frac{dG}{dt} = -k_g G, \quad G(0) = G_0$$
$$\frac{dU}{dt} = k_b B, \quad U(0) = 0$$

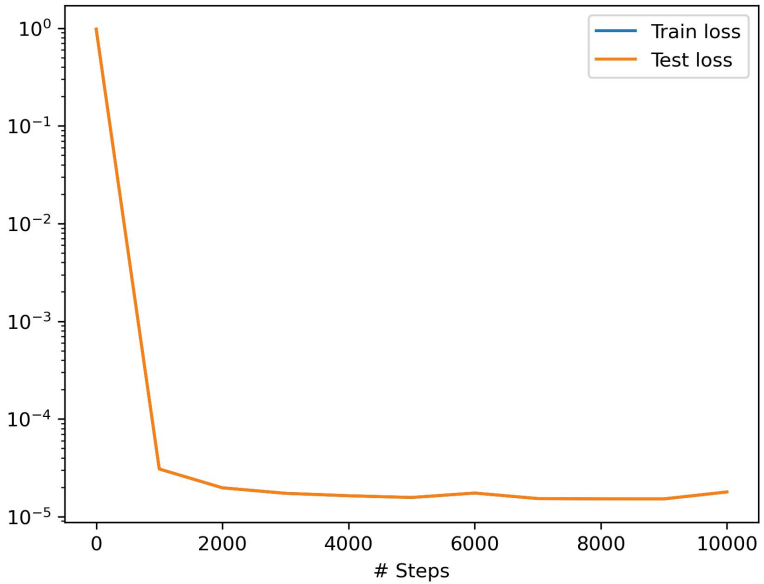


B. Barnes and G. R. Fulford. *Mathematical modelling with case studies: a differential equations approach using Maple and MATLAB.* Chapman and Hall/CRC, 2011.

Basic Forward Problem

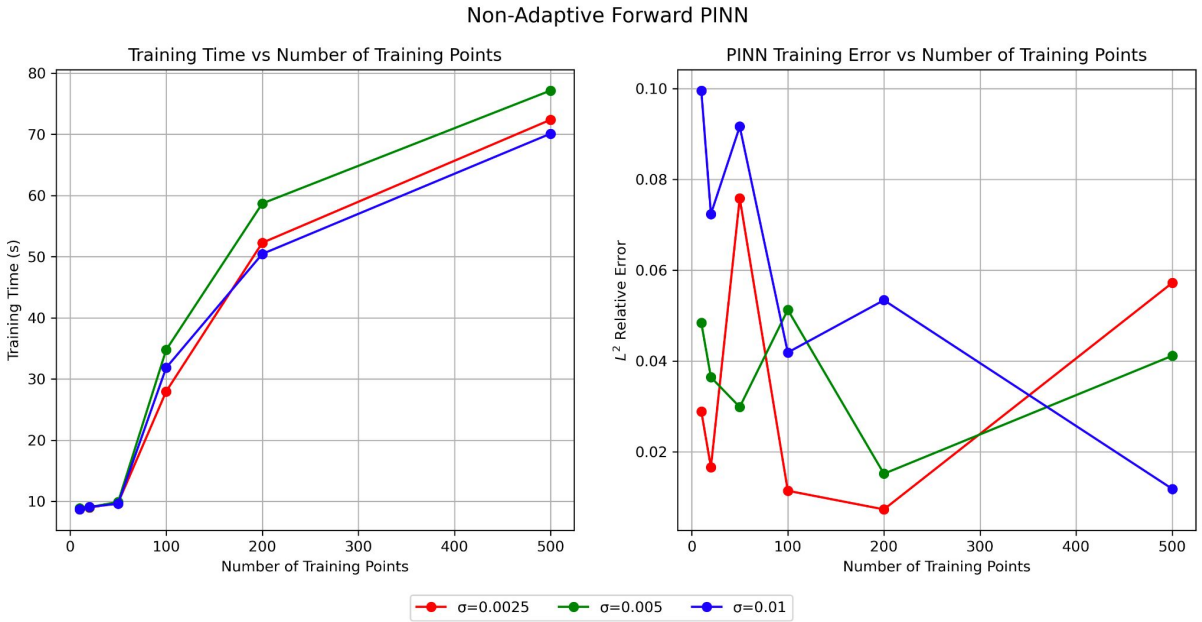
PINN Features: 1 input (t), 2 HLs of 32 neurons, 3 outputs (G, B, U), σ = tanh, 10000 iterations, Adam (lr = 0.001)





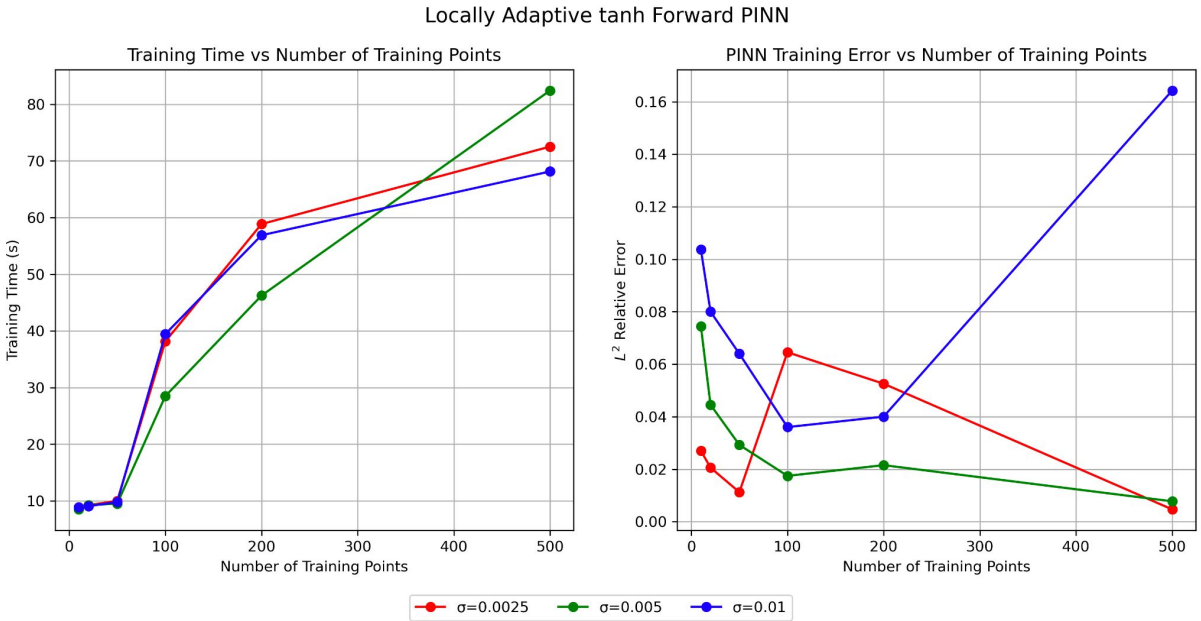
Training Points: 10, 20, 50, 100, 200, 500

Basic Forward Problem



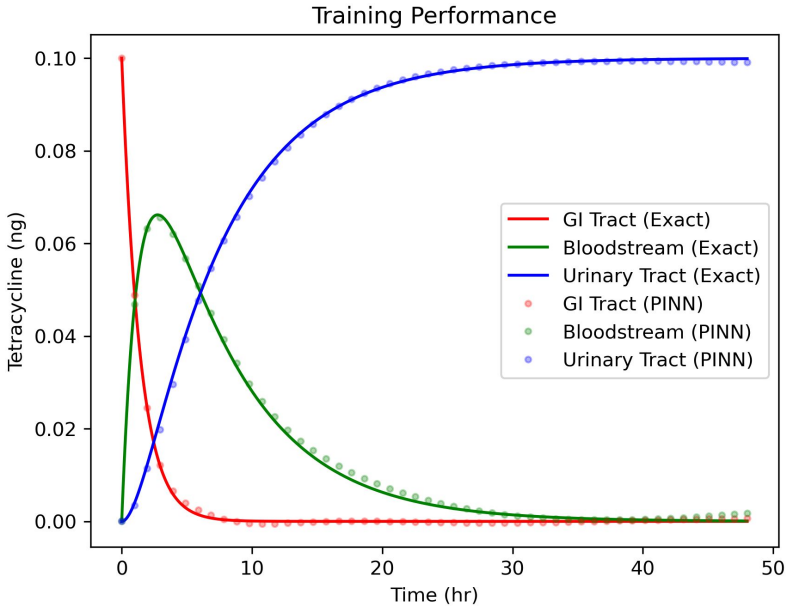
Training Points: 10, 20, 50, 100, 200, 500

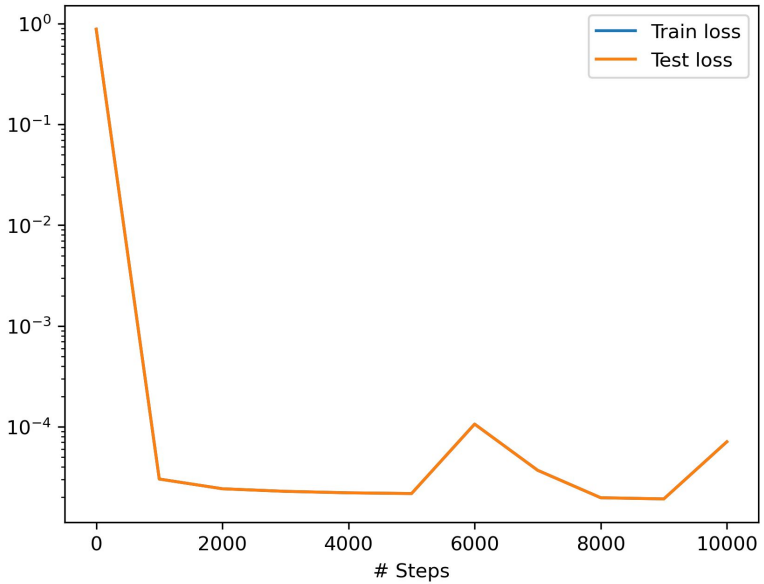
Forward Problem + Locally Adaptive tanh



Basic Inverse Problem

PINN Features: 1 input (t), 2 HLs of 32 neurons, 3 outputs (G, B, U), σ = tanh, 10000 iterations, Adam (lr = 0.001)





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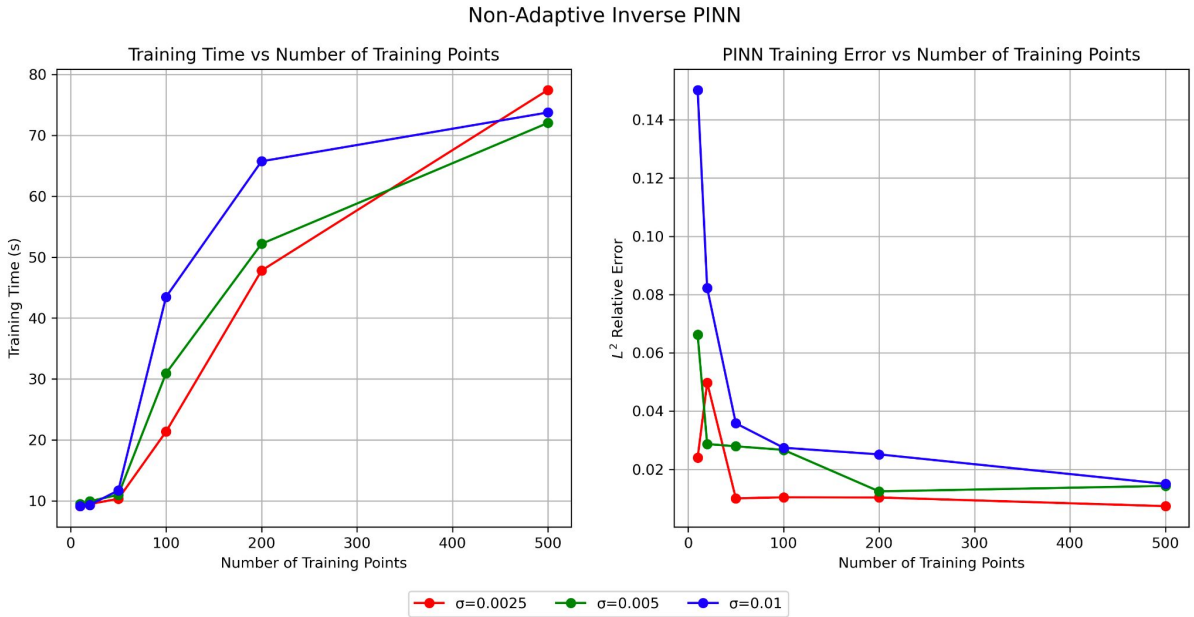
Basic Inverse Problem



Training Points: 10, 20, 50, 100, 200, 500

Inverse Problem + Locally Adaptive tanh