Influence of the Jacobian spectrum on the accuracy of neural network approximation of chemical kinetics

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In this work, a neural network was trained to reproduce the temporal evolution of a hydrogen–oxygen mixture, generated using a reduced chemical kinetic mechanism. After training, the prediction errors (MSE) were analyzed over the test dataset, and the trajectories were divided into percentile groups according to the neural network error. For each percentile group, the local Jacobian matrix of the original kinetic system was reconstructed along the corresponding trajectories and the eigenvalues were used to find the local stiffness of the governing equations. The largest eigenvalues, associated with fast radical reactions, remain in a narrow range of 10^{15}-10^{17} for both well- and poorly-predicted samples. For accurately predicted trajectories, the smallest eigenvalues are typically of order 10^4, resulting in stiffness ratios in the range 10^7-10^{14}. In contrast, for poorly predicted trajectories, the smallest eigenvalues decrease to 10^{-2}-10^1, shifting extreme stiffness ratios up to 10^{16}-10^{21}.

This results demonstrates that the spectrum of the Jacobian has an impact on neural network errors and the magnitude of the smallest eigenvalues can be used as an indicator of cases where models are expected to lose predictive accuracy.

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