METHOD FOR DETERMINING INFORMATIVE PARAMETERS IN NEURAL NETWORK MODELING OF CHEMICAL KINETICS

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The problem of approximating the temporal evolution of a hydrogen–oxygen mixture using a neural network is considered. A fully connected network with 5 layers and LeakyReLU activation was used, trained with Adam (lr = 0.01, 100 epochs) on MSE. Both the input and output of the neural network are vectors comprising the time step Δt, the system temperature, and the molar concentrations of 11 chemical species, with relevant parameter ranges: $T \in [250, 5000]$ K, $p \in [10^4, 2 \times 10^7]$ Pa, and $\Delta t \in [10^{-10}, 10^{-5}]$ s.

Analysis of the test trajectories revealed significant heterogeneity in the error. For the groups with minimal and maximal errors, the spectrum of the Jacobian of the original system was studied. It was found that the key difference is associated with the minimal eigenvalues: for well-approximated trajectories, $\lambda_{\min}$ is on the order of 10^4, while for poorly approximated ones, $\lambda_{\min}$ ranges from 10^{-2} to 10^1. Small $\lambda_{\min}$ values are caused by slow reactions (small k), low concentrations, and quasi-steady-state balancing of forward and reverse reactions. Therefore, the model error is determined by the regimes of the predicted profiles.

Based on this identified relationship, a modification of the loss function is proposed. In addition to the standard MSE term, an additional term is introduced that accounts for the discrepancy between predicted and true values of the logarithms of reaction rate constants, computed using the Arrhenius formula from the predicted temperature.

Comparison of different training variants shows: baseline model: MSE = 1.374×10^{-3}, STD = 2.183×10^{-2}; using all rate constants: MSE = 6.554×10^{-2}, STD = 8.211×10^{-2}; using the selected subset of constants associated with the formation of the slow modes of the system: MSE = 6.482×10^{-4}, STD = 9.308×10^{-3}.

It is shown that the inclusion of a physically informed term in the loss function is effective only with a targeted selection of reactions. Using all constants leads to a deterioration of model quality, whereas considering the reactions that determine slow modes results in more than a twofold reduction in error compared to the baseline approach.

Thus, spectral analysis of the Jacobian can serve as a tool for identifying informative kinetic parameters in neural network modeling of chemical kinetics.

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