Assignment: Neural ODEs for Chemical Kinetics Simulations

Background

You are provided with both training and testing time-series datasets for a chemical reaction. These datasets record the temporal evolution of chemical species and temperature, similar to the systems analyzed in the ChemNode research paper. The testing dataset represents a chemical reaction with a different initial condition to that of training data.

Note: While the ChemNode paper focuses on hydrogen combustion, your assignment uses the **GRI v3.0 mechanism**, which models methane combustion. The underlying modeling approaches and analysis remain similar, but the reaction mechanism is different.

Following is a breakdown of the tasks and deliverables:

1. Literature Review

- Go through the provided Neural ODE tutorial repository to understand the neural ODE framework.
- Go through the ChemNode research paper. You will need to solve the same problem on different inputs.

2. Model Design & Implementation

- Design and implement your own model or algorithm to predict the time evolution of the system (for all or selected species), grounded in insights from the ChemNode approach.
- **Use a neural ODE approach.** Your choice of loss function or model architecture may differ from that in the ChemNode paper—that is encouraged!
- You are not required to exactly reproduce the ChemNode method, but your solution should be scientifically motivated and aim for comparable predictive results.
- You may utilize standard Python libraries for numerical ODE solvers.

3. Evaluation & Comparison

- Test your trained model's predictive capability on the provided testing dataset.

- Evaluate the accuracy of your model's predictions on both the training and testing datasets using suitable quantitative metrics (e.g., MAE, RMSE, or custom metrics found in the ChemNode paper).
- Compare your model's results with those highlighted in the ChemNode paper and discuss similarities or differences.

4. Reporting

- Submit the following:
    - Your fully documented code (as a script or notebook), with clear instructions for running your solution.
    - Plots for your model evaluation. Comparision of testing data with pridicted data for several important species from mechanism (CH4, H2O, O2 etc) and temperature.
    - Report clearly describing your approach, rationale, results, and interpretations.

Resources

- The ChemNode paper (Link provided), as well as both the training and testing datasets, are included in the ZIP folder you received via email.
- Neural ODE tutorial and starter code

Hint

- **Carefully study the pseudocode and workflow described in the ChemNode paper.** Pay close attention to how inputs and outputs are defined for the neural ODE setup, and how the error (loss) function is constructed—specifically, whether it is computed directly on the neural network's output or elsewhere in the pipeline.
- **Remember:** Neural ODE architectures are structurally different from standard neural networks. Focus on understanding the distinction between how typical neural networks are trained and how neural ODEs are formulated, solved, and optimized.

If you need clarification on any point, please feel free to ask before the assignment deadline.