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Understanding the latent manifolds of autoencoders using information geometry for the stiff dynamical systems

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Efficient computation of finite-rate chemical kinetics remains a critical challenge in modern reacting flow simulations due to inherent system stiffness. Building upon our previous research, which introduced the dynamic-informed training methodology to mitigate stiffness in chemical dynamics. The proposed combined autoencoder and neural ordinary differential equation approach effectively eliminates stiffness, relaxing the time step requirements. The autoencoder facilitates the computation of an optimized low-dimensional latent space. However, the principle behind this process remains to be explored. Due to this, the combined neural network is treated as a black box. Recognizing the latent space as a curved manifold with curvilinear coordinates, simple tools from Riemann geometry are employed for the analysis. In this work, information geometry is utilized to unveil the geometric structure of the latent variables corresponding to the physical state variables. This helps to understand the latent manifold formulation during the training process. The necessary degrees of freedom for describing the chemical dynamics are also accurately determined. The findings contribute to a deeper understanding of the neural network-based reduced order models, aiding in more efficient computational modeling of reacting flow systems.

Keywords: Chemical kinetics, reduced order model, neural ODE, autoencoder, information geometry