Visualizing the energy landscape of glassy systems

Vaibhav Bihani*[1], Srikanth Sastry[2], Sayan Ranu[1], and Anoop Krishnan N M†[1]

[1]Indian Institute of Technology Delhi – India
[2]Jawaharlal Nehru Centre for Advanced Scientific Research – India

Abstract

Understanding the energy landscape is key to discovering glasses with targeted properties since the landscape encapsulates a system's complete thermodynamic and kinetic behavior, including its non-equilibrium properties, such as relaxation and metastable phases. However, the curse of dimensionality prohibits one from effectively visualizing the energy landscape-the energy landscape of an N-atom system has 3N dimensions. Here, we propose a method to visualize the complex energy landscape. We demonstrate that the proposed low-dimensional projection aligns well with the curvatures of the actual landscape, validated through Hessian analysis. Further, we show that we can gain interesting insights into the behavior of different gradient-based and machine-learned optimizers using the proposed visualization approach. Through this study, we aim to enhance comprehension of energy landscapes and contribute to a fundamental understanding of the physics underlying glassy materials. Furthermore, we anticipate that our method will expedite the discovery process of these materials.

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*Speaker
†Corresponding author: krishnan@iitd.ac.in