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Building better biomolecular physics models with differentiable simulation

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Developing physics-based models for molecular simulation requires fitting many unknown parameters to experimental datasets of diverse properties. Model development typically proceeds according to the trial-and-error tinkering of individual researchers, and the procedures by which parameters are chosen are often opaque and irreproducible. This erects significant barriers to extending and improving existing models –for example, refitting parameters to new experimental data –leading to redundant models of nucleic acids and protein, as developing a new model from scratch is often easier than tweaking extant models. In this talk, I'll highlight how my collaborators and I are leveraging machine learning tools –namely, gradient estimates with automatic differentiation –to facilitate the extensible, reproducible, and transparent fitting of the physics-based DNA model oxDNA. We have developed a differentiable nucleic acid model: jaxDNA, which I'll use to illustrate simultaneous parameter fitting to multiple loss functions, spanning structural, mechanical, and thermodynamic data. Our framework can also be used to 'reverse engineer'DNA systems, and I'll show results for inverse DNA sequence design. Finally, I'll demonstrate how our open-source jaxDNA framework can be used to customize models and objective functions. Though grounded in oxDNA, our work provides a general framework for extensible, community-driven force field development we hope will lead to improved models for systems ranging from RNA to proteins.

Keyword-1

nucleic acid model

Keyword-2

differentiable simulation

Keyword-3

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