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Perspective

# Challenges of Biomolecular Modeling with Machine Learning and Artificial Intelligence

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## DESCRIPTION

Biomolecular modeling is a field that uses computational methods to study the structure, function and interactions of biological molecules such as proteins DNA and RNA. Machine Learning (ML) and Artificial Intelligence (AI) are fields that use algorithms to learn from data and perform tasks that require human intelligence such as classification prediction and decision making. Integrating biomolecular modeling with ML and AI can offer many opportunities to advance the understanding and engineering of biological systems but also ome challenges that need to be addressed. One of the opportunities of integrating biomolecular modeling with ML and AI is to enhance the accuracy and efficiency of biomolecular simulations. Biomolecular simulations are based on physics-based models that describe the interactions and motions of atoms and molecules. However these models have limitations in terms of accuracy scalability and transferability. For example the force fields that define the potential energy of a system may not capture all the relevant effects or may be parameterized for a specific system.

ML and AI can help improve the force fields by learning from experimental or quantum mechanical data and incorporating non-linear or adaptive features. ML and AI can also help reduce the computational cost of biomolecular simulations by learning coarse-grained models that represent groups of atoms as single entities or by learning surrogate models that approximate expensive calculations. Another opportunity of integrating biomolecular modeling with ML and AI is to discover new insights and hypotheses from large and complex biomolecular data. Biomolecular data are generated from various sources, such as experiments, simulations, databases and literature. These data are often heterogeneous, incomplete or high-dimensional. ML and AI can help analyze and integrate these data by applying techniques such as dimensionality reduction, clustering, classification, regression, feature selection and network analysis. ML and AI can also help generate new data or models by applying techniques such as generative adversarial networks, variation reinforcement learning and inverse design. These techniques can help discover novel structures, functions, interactions or pathways of biomolecules that can inspire new experiments or applications.

However, integrating biomolecular modeling with ML and AI also faces some challenges that need to be overcome. One of the challenges is to ensure the validity and reliability of the ML and AI models. ML and AI models are often based on empirical or statistical assumptions that may not reflect the underlying physical or biological principles. For example ML and AI models may over fit the training data or extrapolate beyond the domain of applicability. Therefore it is important to validate the ML and AI models using independent data or benchmarks and to quantify their uncertainties and errors. It is also important to interpret the ML and AI models using explainable or interpretable methods that can reveal the underlying mechanisms or causal relationships. Another challenge is to foster the collaboration and communication between different disciplines involved in integrating biomolecular modeling with ML and AI. Biomolecular modeling requires expertise in fields such as chemistry, biology physics and mathematics. ML and AI require expertise in fields such as computer science, statistics and engineering. Integrating these fields requires a common language and framework that can bridge the gap between different concepts, methods and tools. It also requires a culture of openness and sharing that can facilitate the exchange of data, models and knowledge.

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