

cases	doc_1		doc_2		decision	id
	authors	<ul style="list-style-type: none"><li>Ying Tang</li><li>Jiayu Weng</li><li>Pan Zhang</li></ul>	authors	<ul style="list-style-type: none"><li>Tang, Ying</li><li>Weng, Jiayu</li><li>Zhang, Pan</li></ul>	DUPLICATES	198
	title	Neural-network solutions to stochastic reaction networks	title	Neural-network solutions to stochastic reaction networks		
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	id	id5036769134676410724	id	id1715864676350460193		
	abstract	The stochastic reaction network in which chemical species evolve through a set of reactions is widely used to model stochastic processes in physics, chemistry and biology. To characterize the evolving joint probability distribution in the state space of species counts requires solving a system of ordinary differential equations, the chemical master equation, where the size of the counting state space increases exponentially with the type of species, making it challenging to investigate the stochastic reaction network. Here, we propose a machine-learning approach using the variational autoregressive network to solve the chemical master equation. Training the autoregressive network employs the policy gradient algorithm in the reinforcement learning framework, which does not require any data simulated in prior by another method. Different from simulating single trajectories, the approach tracks the time evolution of the joint probability distribution, and supports direct sampling of configurations and computing their normalized joint probabilities. We apply the approach to representative examples in physics and biology, and demonstrate that it accurately generates the probability distribution over time. The variational autoregressive network exhibits a plasticity in representing the multimodal distribution, cooperates with the conservation law, enables time-dependent reaction rates, and is efficient for high-dimensional reaction networks with allowing a flexible upper count limit. The results suggest a general approach to investigate stochastic reaction networks based on modern machine learning.	abstract	The stochastic reaction network is widely used to model stochastic processes in physics, chemistry and biology. However, the size of the state space increases exponentially with the number of species, making it challenging to investigate the time evolution of the chemical master equation for the reaction network. Here, we propose a machine-learning approach using the variational autoregressive network to solve the chemical master equation. The approach is based on the reinforcement learning framework and does not require any data simulated in prior by another method. Different from simulating single trajectories, the proposed approach tracks the time evolution of the joint probability distribution in the state space of species counts, and supports direct sampling on configurations and computing their normalized joint probabilities. We apply the approach to various systems in physics and biology, and demonstrate that it accurately generates the probability distribution over time in the genetic toggle switch, the early life self-replicator, the epidemic model and the intracellular signaling cascade. The variational autoregressive network exhibits a plasticity in representing the multi-modal distribution by feedback regulations, cooperates with the conservation law, enables time-dependent reaction rates, and is efficient for high-dimensional reaction networks with allowing a flexible upper count limit. The results suggest a general approach to investigate stochastic reaction networks based on modern machine learning		
	versions		versions			