Deep neural cellular Potts models

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Abstract

The cellular Potts model (CPM) is a powerful computational method for simulating collective spatiotemporal dynamics of biological cells. To drive the dynamics, CPMs rely on physics-inspired Hamiltonians. However, as first principles remain elusive in biology, these Hamiltonians only approximate the full complexity of real multicellular systems. To address this limitation, we propose NeuralCPM, a more expressive cellular Potts model that can be trained directly on observational data. At the core of NeuralCPM lies the Neural Hamiltonian, a neural network architecture that respects universal symmetries in collective cellular dynamics. Moreover, this approach enables seamless integration of domain knowledge by combining known biological mechanisms and the expressive Neural Hamiltonian into a hybrid model. Our evaluation with synthetic and real-world multicellular systems demonstrates that NeuralCPM is able to model cellular dynamics that cannot be accounted for by traditional analytical Hamiltonians.