Learning dynamical processes on complex networks from time series

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Dynamical processes on real complex networks are typically accessed by time series of the state of every node [1]. A popular strategy to further our understanding of these underlying complex mechanisms is to develop mechanistic representations of these phenomena—simple dynamical models. While they offer useful, often mathematical, insights [2], they usually lack effective predictive power. The reason is that these real phenomena can hardly be represented by such simplistic representations, and more complex representations are needed to provide better predictions. In this vein, we consider the problem of *learning* dynamical processes on complex networks from actual time series data using deep learning (see Fig. a). We show that this multivariate time series forecasting (MTSF) task can scarcely be successfully learned by standard machine learning approaches [3]. This is due in part to the lack of structural information encompassed by these models, for which the state of each node depends directly on the state of every other nodes. Inspired by recent advances in deep convolutional neural networks, we develop a conditional variational auto-encoder (CVAE) framework that takes such structural information into account explicitly. Instead of connecting the present state of each node to the past states of every node in the network within the CVAE, similarly to standard MTSF approaches, we consider a different CVAE for each individual node. Then, each model conditions the present state of its node only on its past states and those of its neighbors with shared parameters (see Fig. b). Using non-markovian variations of the *Susceptible-Infected-Susceptible* dynamics, we show that our approach allows the generative model to learn more effectively the dynamical rules between nodes than standard MTSF approaches. By doing so, we develop a proof of concept, in line with Ref. [4] but in the realm of complex networks, which advocates the use of machine learning for predicting real complex network dynamics.

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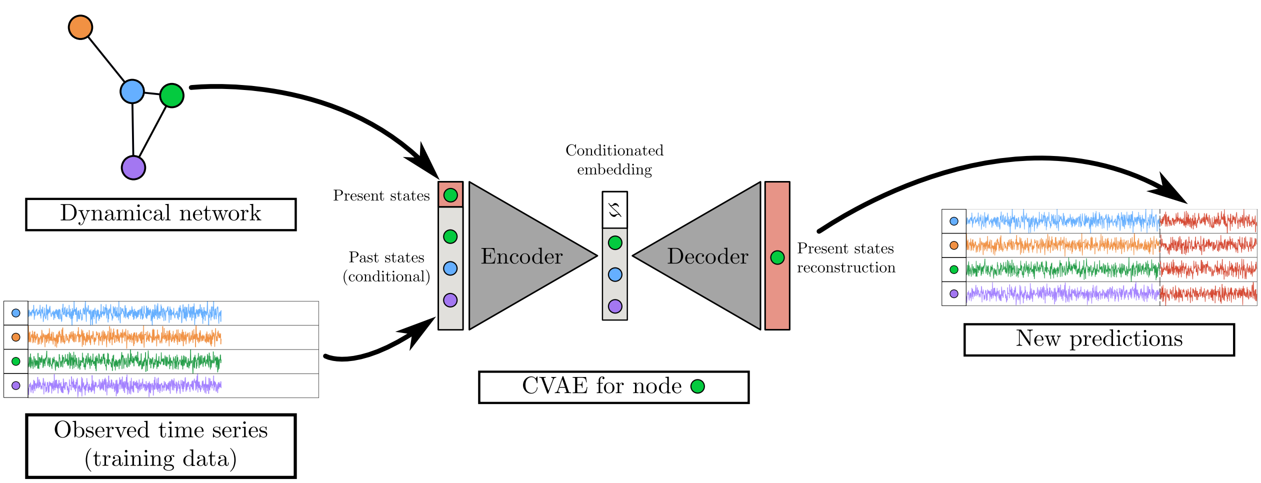

Figure: Illustration of the procedure for learning dynamics on complex networks with CVAEs. We use the time series of the state of each node of a dynamical network to train an unsupervised CVAE. These CVAEs use encoders—deep neural networks—that map the present state of a node into a distribution over an embedding, z, conditioned over the past states of this node and those of its neighbors. This embedding is then fed to a decoder—another deep neural network—to reconstruct the node present state. After training, one can generate new predictions of the node states over time by sampling z conditioned on the neighbors past states and feeding it through the decoder.