Title of the work program

Generative approach to complex random walks

Description of the work program

We have recently introduced a simulation-based, amortised Bayesian inference scheme to infer the parameters of random walks[1]. Our approach learns the posterior distribution of the walks' parameters with likelihood-free methods[2]. In the first step a graph neural network is trained on simulated data to learn optimised low-dimensional summary statistics of the random walk. In the second step an invertible neural network generates the posterior distribution of the parameters from the learnt summary statistics using variational inference[3].

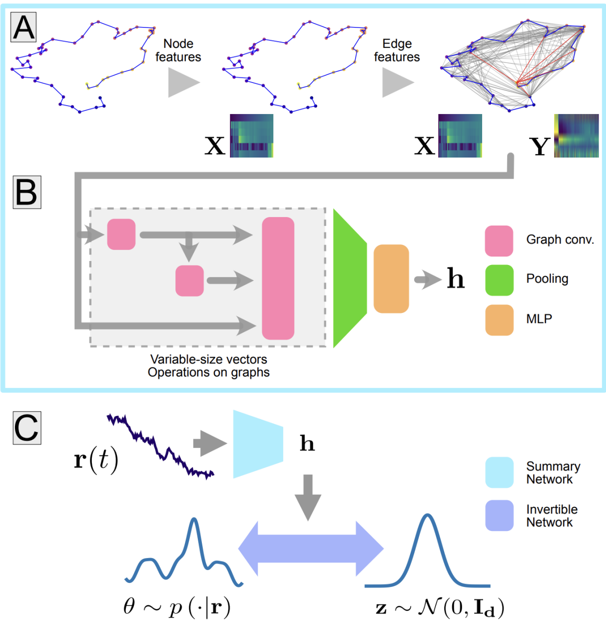

FIG. 1. Model Architecture. A: Construction of a graph from a single trajectory (left). Positions, colored according to time, are treated as nodes for which features X are computed (middle). Nodes are then connected by edges (grey lines) following a given wiring scheme, and edge features Y are computed. Edges terminating at the trajectory's last point are shown in red. Feature matrices for both nodes (X) and edges (Y) are depicted in small insets with colour coded values. B: Summary network extracting information from the trajectory's graph. It consists of several graph convolution layers (in purple), a pooling layer (green) and a multi-layer perceptron (orange). The vector of statistics it outputs is indicated by h. C: General structure of the model, with the summary network (light blue) extracting from the trajectory r(t) the summary statistics vector h, which in turn parameterised the invertible network. During the training phase, the invertible network is used from left to right (i.e., from the parameter's manifold to an easily sampled one), and in inference mode it is used from right to left.

We applied our method to infer the parameters of the fractional Brownian motion model from single trajectories[1]. The computational complexity of the amortised inference procedure scales linearly with trajectory length[4], and its precision scales similarly to the Cramer-Rao bound over a wide range of lengths. The approach is robust to positional noise[5], and generalises to trajectories longer than those seen during training. We extended our method to random walks lacking Green functions and applied it to experimental recordings of neural receptor in and out of synapses[6]

In this internship we seek to build on our recent advances to devise a generative model of complex random walks starting with anomalous diffusion. We will leverage the current network architecture and denoising diffusion probabilistic models[7] to attempt to generate these random walks. Beyond being able to properly generate canonical models, which will already be an achievement, we seek to explore the diversity of random walks properties generated by these approaches.

Tutors/supervisors

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Selected publications

1. Verdier, H., Laurent, F., Vestergaard, C., Cassé, A. & Masson, J.-B. Amortised inference of fractional Brownian motion with linear computational complexity. *arXiv:2203.07961 [physics, q-bio]* (2022).
2. Cranmer, K., Brehmer, J. & Louppe, G. The frontier of simulation-based inference. *PNAS* **117**, 30055–30062 (2020).
3. Radev, S. T., Mertens, U. K., Voss, A., Ardizzone, L. & Kothe, U. BayesFlow: Learning Complex Stochastic Models With Invertible Neural Networks. *IEEE Trans. Neural Netw. Learning Syst.* 1–15 (2020) doi:10.1109/TNNLS.2020.3042395.
4. Verdier, H. *et al.* Learning physical properties of anomalous random walks using graph neural networks. *J. Phys. A: Math. Theor.* **54**, 234001 (2021).
5. Muñoz-Gil, G. *et al.* Objective comparison of methods to decode anomalous diffusion. *Nat Commun* **12**, 6253 (2021).
6. Verdier, H. *et al.* A maximum mean discrepancy approach reveals subtle changes in α-synuclein dynamics. 2022.04.11.487825 Preprint at https://doi.org/10.1101/2022.04.11.487825 (2022).
7. Ho, J., Jain, A. & Abbeel, P. Denoising Diffusion Probabilistic Models. *arXiv:2006.11239 [cs, stat]* (2020).

Scientific or technical background required for work program

The interested student should either
- be a physicist with knowledge in generative deep learning
- be an applied mathematician interested in physics random walks