Manifold rewiring for unlabeled imaging in large noise

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In X-ray tomography the task is to reconstruct an unknown density from its projections in a number of directions. Stable recovery requires a sufficient number of projections and the knowledge of the relative projection angles. In some applications, however, projection angles are unknown; an important example is single-particle Cryo-EM. With small or moderate noise it is relatively straightforward to infer the viewing directions in Cryo-EM [1]. As the noise increases, direction recovery becomes hard. We propose a general graph-learning framework to recover unknown parameters in Cryo-EM-like problems where the unknown quantity (such as viewing direction) has a manifold structure.

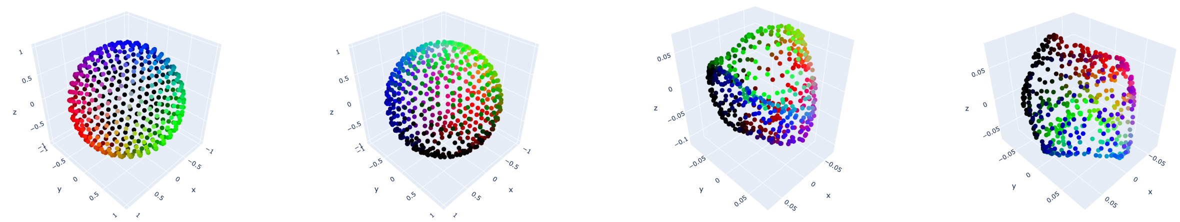
Concretely, let $\mathcal{M}$ denote a smooth manifold and $\mu \in \mathcal{P}_1(\mathcal{M})$ a probability measure on $\mathcal{M}$. We observe (very) noisy measurements through a function $f : \mathcal{M} \to \mathbb{R}^N$,

$$y_i = f(\theta_i) + \eta_i, \tag{1}$$

where $\theta_i \overset{i.i.d.}{\sim} \mu$, and $\eta_i \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2 \mathrm{I}_N)$ is a Gaussian random vector. Put differently, we observe $y_i \overset{i.i.d.}{\sim} \nu$ where $\nu \overset{\text{def.}}{=} f_{\#}\mu \star \mathcal{N}(0, \sigma^2 \mathrm{I}_N)$, $f_{\#}\mu$ denotes the pushforward of μ by f, and $\star$ is the convolution of measures.

Fig. 1 shows an embedding of 3D Cryo-EM projections. The underlying metric quotients out the so-called in-plane rotations so the embedding lives on $\mathbb{SO}(3)/\mathbb{S}^1 \simeq \mathbb{S}^2$ rather than $\mathbb{SO}(3)$ [2]. The function f corresponds to the 3D X-ray transform and the underlying manifold is $\mathcal{M} = \mathbb{S}^2$, see Fig. 1a. In the absence of noise, the parameters $(\theta_i)_i$ on the sphere can be deduced from the graph Laplacian embedding of the measurements $(y_i)_i$; Fig. 1b. For large noise, the graph Laplacian embedding collapses and the relative position of the observation cannot be deduced; Fig. 1c.

This is because the noisy neighborhood graph contains false and misses true links. We propose to use the recent WalkPooling neural network architecture [3] to denoise the K-NN graph. The WalkPooling architecture captures the topological properties of $\mathcal{M}$ by learning to construct graphs from points sampled from the distribution μ. This leads to significant improvements in embedding quality and enables reconstruction at extreme noise levels; Fig. 1d.



(a) Underlying manifold: S^2. (b) Noiseless embedding. (c) Noisy embedding(0dB). (d) WalkPooling (0dB).

Figure 1: Single particle 3D cryo-EM motivation example: the measurments are function of parameters in S^2. The Graph-Laplacian embedding allows to retrieve the relative position of each projection only using WalkPooling to denoise the graph.

Joint work with: Ivan Dokmanić, Vinith Kishore, Cheng Shi.

References

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