Application of Graph Learning to inverse problems

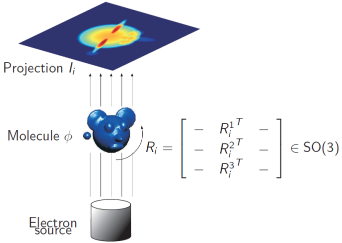
Cédric Mendelin <cedric.mendelin@stud.unibas.ch>

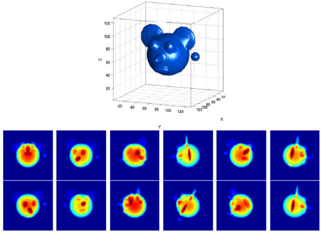
Department of Mathematics and Computer Science, University of Basel

Date

Outline

Cryo-EM





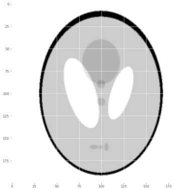
Cryo-EM overview Singer 2018, Figure 1 and Figure 2

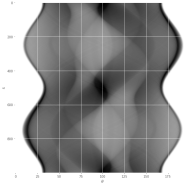
Cryo-EM challenges

- High-noise level
- Unknown rotation during freezing
- (Structural variety of observations)

The main domain of interest is the high-noise domain (cryo-EM).

Computed Tomography





- Related to cryo-EM
- Can be seen as simpler version in 2D
- Good to start with

Graph construction

Let Ω be a dataset $\Omega \subset \mathbb{R}^M$, a graph can be constructed like:

- V: each node associated with $x \in \Omega$
- E: Calculate adjacency matrix with similarity measure d and some threshold τ

Definition (Adjacency Matrix)

$$A_{ij} = \begin{cases} 1 & \text{if } d(x_i, x_j) < \tau \\ 0, & \text{otherwise} \end{cases} \tag{1}$$

Graph construction

Let Ω be a dataset $\Omega \subset \mathbb{R}^M$, but only observation of $y = x + \eta$ (with η drawn from $\mathcal{N} \sim (0, \sigma^2)$), a graph can be constructed like:

- V: each node associated with $y \in \Omega$
- E: Calculate adjacency matrix with similarity measure d and some threshold τ

Definition (Noisy Adjacency Matrix)

$$A_{0_{ij}} = \begin{cases} 1 & \text{if } d(y_i, y_j) < \tau \\ 0, & \text{otherwise} \end{cases} \tag{2}$$

Noisy graph

Theorem

For every noisy graph $G_0 = \langle V, E_0 \rangle$, there exists a noiseless graph $G = \langle V, E \rangle$. Both graphs consists of the same set of vertices V but different edges. E_0 is defined as follows:

$$E_0 = E \setminus E_0^- \cup E_0^+,$$

where $E_0^- \subseteq E$ and $E_0^+ \subseteq U$ with U the set of all possible edges and $E_0^+ \cap E = \emptyset$

Graph Denoising

Graph denoising is the task, to estimate a denoised graph $\tilde{G}$ from a given noisy graph G_O, with underlying original graph G:

Definition (Graph Denoising)

$$GD : G_0 \mapsto \tilde{G} \approx G,$$

where G_0, $\tilde{G}$, G denotes noisy, estimated denoised and original graph respectively.

Definition (Graph Denoising)

$$GD : A_0 \mapsto \tilde{A} \approx A,$$

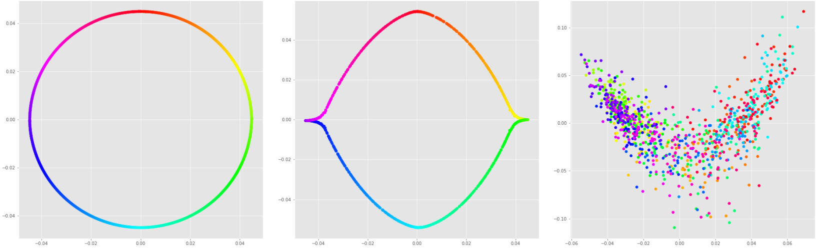
where A_0, $\tilde{A}$, A denotes adjacency matrix from G_0, $\tilde{G}$ and G respectively.

Manifolds

We know structure of manifolds for noiseless data:

- Computed Tomography $\rightarrow$ circle
- Cryo-Em $\rightarrow$ sphere

If data is noisy, manifold will "drift" away from noiseless manifold:

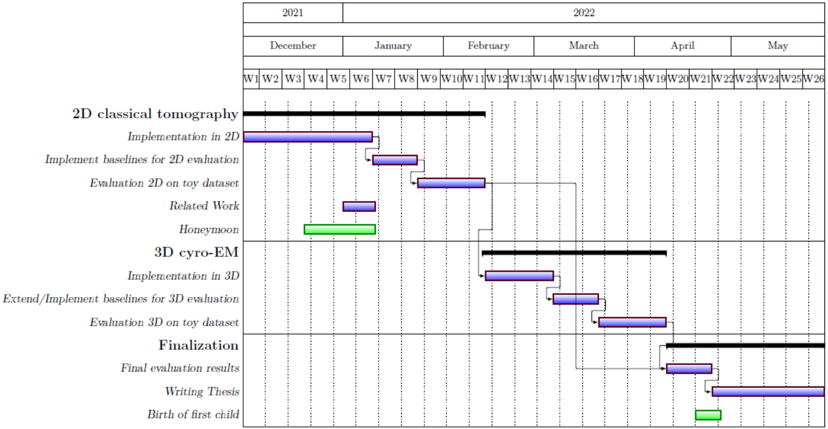


Manifolds for phantom without noise, and different noise levels.

Project Conclusion

- Introduce Graph Denoising method
- Focus on high-noise domain (cryo-EM)
- Exploit known manifold in 2D and 3D
- Further study Graph Laplacian and connection with
  - Tomography domain
  - GNNs and Machine Learning in general
- Evaluate on toy dataset in 2D and 3D
- Nice to have: evaluate on cryo-EM / CT dataset

Project schedule



Questions?

References

- Singer, Amit (2018). “Mathematics for cryo-electron microscopy”. In: **Proceedings of the International Congress of Mathematicians: Rio de Janeiro 2018**. World Scientific, pp. 3995–4014.