Application of Graph Learning to inverse problems

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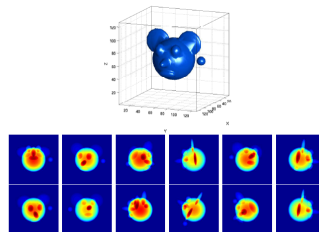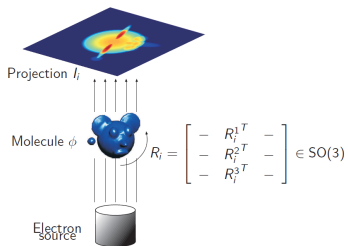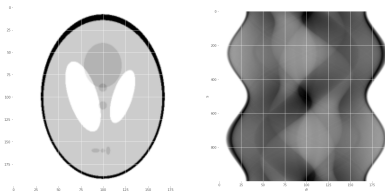
Date

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

Definition (Observation)

$$y_i[j] = R(x, \theta_i, s_j) + \eta_i[j], \text{ with } 1 \le i \le N \text{ and } 1 \le j \le M,$$

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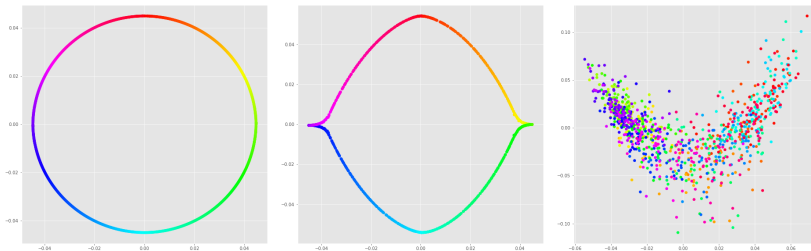
$$GD : A_0 \mapsto \tilde{A} \approx A,$$

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 noise less manifold:
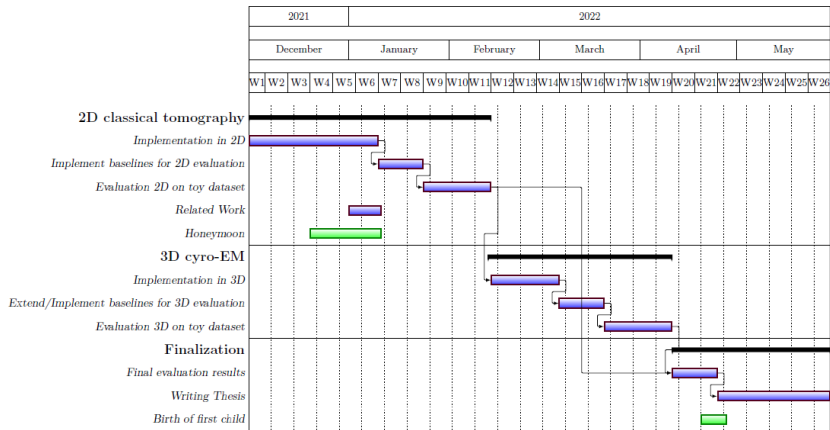

Manifolds for phantom without noise, and different noise levels.

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

	2021	2022				
	December	January	February	March	April	May

2D classical tomography
Implementation in 2D
Implement baselines for 2D evaluation
Evaluation 2D on toy dataset
Related Work
Honeymoon

3D cyro-EM
Implementation in 3D
Extend/Implement baselines for 3D evaluation
Evaluation 3D on toy dataset

Finalization
Final evaluation results
Writing Thesis
Birth of first child

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.