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Application of Graph Learning to inverse problems

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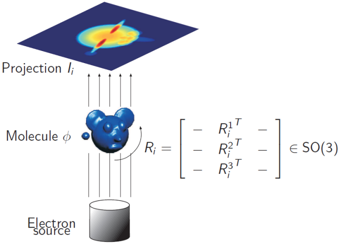
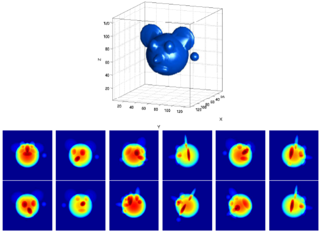
Date

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)

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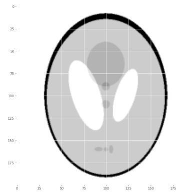
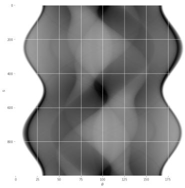
The main domain of interest is high-noise domain (cryo-EM).

Computed Tomography





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

Graph construction

Consider n observed images $(x_0, x_1, \ldots, x_n)$, where $x_i \in \mathbb{R}^M$ with M as image dimension. A graph can be constructed by:

- V: The images can be used as nodes.
- E: If similarity measure d of two images x_i, x_j is smaller than given threshold τ, there will be an edge.

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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

Consider n observed **noisy** images $(y_0, y_1, \ldots, y_n)$, where $y_i \in \mathbb{R}^M$ with M as image dimension. Then, $y_i = x_i + \eta$ with η drawn from $\mathcal{N} \sim (0, \sigma^2)$ and $(x_0, x_1, \ldots, x_n)$ as the original images. A noisy graph can be constructed like:

- V: The **noisy** images y can be used as nodes.
- E: If similarity measure d of two **noisy** images y_i, y_j is smaller than given threshold τ, there will be an edge.

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- V: The **noisy** images y can be used as nodes.
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Definition (Noisy Adjacency Matrix)

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

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.

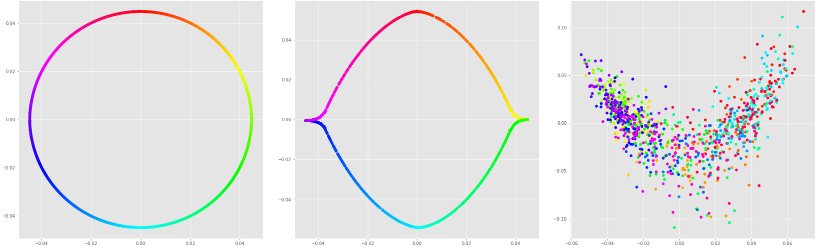
Slide about Manifolds on cryo-EM and CT.

Manifolds

We know structure of manifolds for noiseless data:

- Computed Tomography → circle
- Cryo-Em → sphere

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

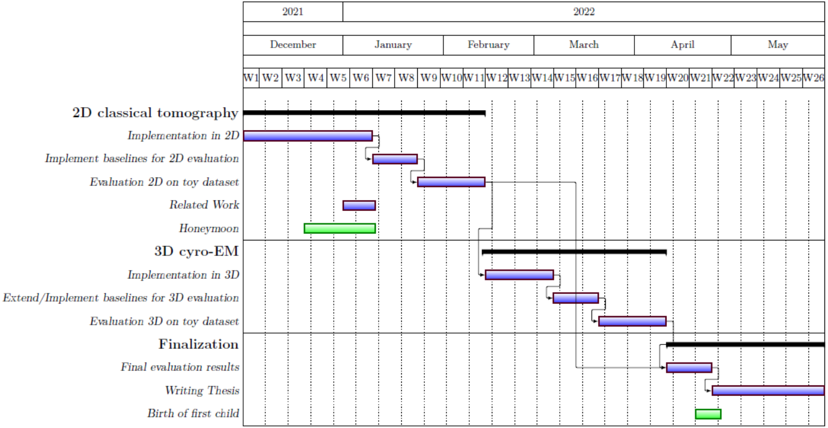


Manifolds for phantom without noise, and different noise levels.

Project Conclusion - Next steps

- Focus on high-noise domain (cryo-EM)
- Introduce Graph Denoising method
- 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.