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Application of Graph Learning to inverse problems

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Date

Outline

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Cryo-electron microscopy (cryo-EM)

- Allows observation of molecules in near atomic resolution.
- Samples are frozen and further observed in electron microscope.
- During freezing, molecules rotates randomly.
- Frozen molecules are fragile, electron microscope needs to work with low power.
- Observations can be reconstructed to 3D model.

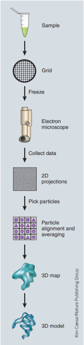

Figure: Cryo-EM workflow Doerr 2016, Figure

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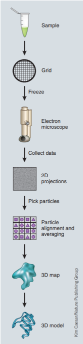
Only single particle cryo-EM is considered.



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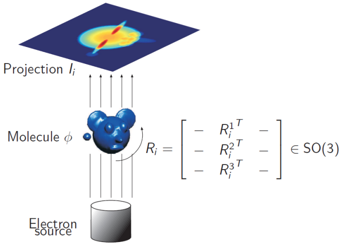
Cryo-EM



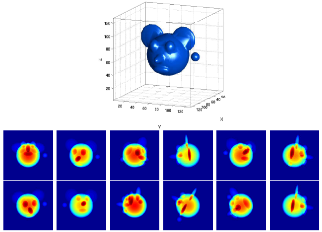


Figure: Cryo-EM overview Singer 2018, Figure 1 and Figure 2

Cryo-EM challenges

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

(a) Noiseless photograph

(b) Noisy photograph

Figure: Noise observation example

Cryo-EM challenges

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

Master Thesis domain of interest is to high-noise regime (cryo-EM). Goal is to introduce a denoise method for cryo-EM 2D projections.

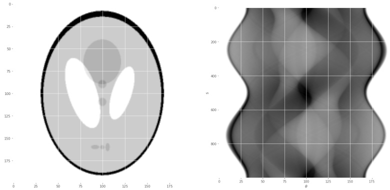
(a) Noiseless photograph

(b) Noisy photograph

Figure: Noise observation example

Computed Tomography

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



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Graph construction

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

- V: 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: **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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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.

Outline

Abstract model without noise

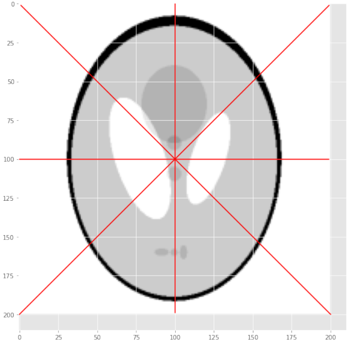
Definition

$$y_i = A(x, \theta_i), \text{ with } 1 \leq i \leq N,$$

- $\Omega \subset \mathbb{R}^D$ as original object space with dimension D
- $\tilde{\Omega} \subset \mathbb{R}^{D-1}$ as observations space with dimension $D-1$.
- $y_i \in \tilde{\Omega}^M$ with M observation dimension
- $x \in L^2(\Omega)$
- $\theta_i \in \mathbb{R}^P$ projection angle vector with projection dimension P
- $A : L^2(\Omega) \to L^2(\tilde{\Omega}), x \mapsto A(x; \theta_i)$, a non-linear operator

Computed tomography - low-dimensional manifold

- Observations y_i with angle θ_i
- There is a mapping between observation y_i and θ_i
- For computed tomography, $\theta \in [0, 2\pi]$ (circle)
- Therefore, there exists a one to one mapping from y_i to point on the circle $(\cos\theta_i, \sin\theta_i)$.



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:

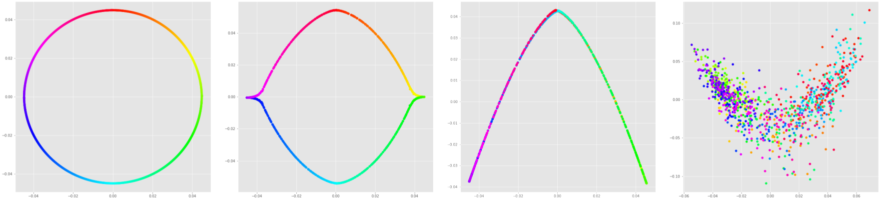
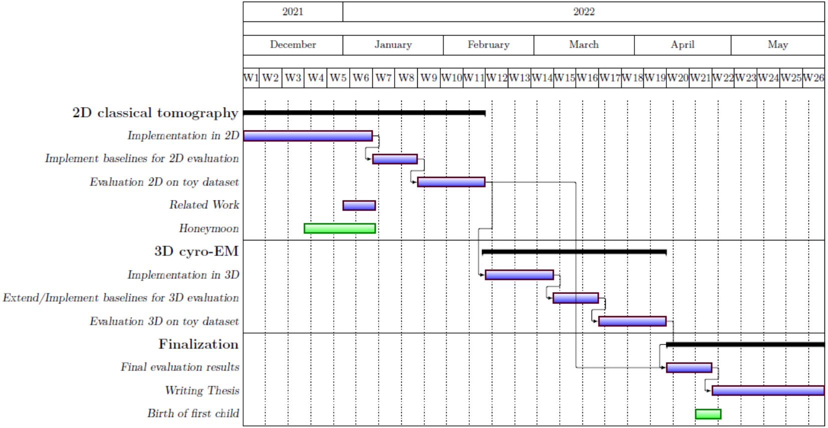


Figure: Manifolds for phantom without noise, and different noise levels.

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

- Doerr, Allison (2016). "Single-particle cryo-electron microscopy". In: **Nature methods** 13.1, pp. 23–23.
- 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.