Graph Denoising for Molecular Imaging

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Outline

Signal-to-noise-ration (SNR)

Reconstruction

SNR is a measure, which compares the power of an input signal to the power of the undesired noise.

Outline

Cryo-Electron Microscopy (Cryo-EM)

- Enables observation of molecules in near atomic resolution.
- Major motivation for Thesis.
- During freezing, molecules rotate randomly.
- Frozen molecules are fragile, electron microscope needs to work with low power.
- Observations can be reconstructed to 3D model.

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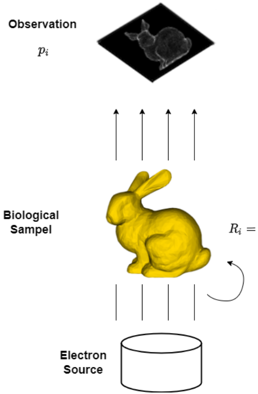
Only single particle cryo-EM is considered.

Cryo-EM



$$R_i = \begin{bmatrix} - & R_i^{1^T} & - \\ - & R_i^{2^T} & - \\ - & R_i^{3^T} & - \end{bmatrix} \in SO(3)$$

Cryo-EM

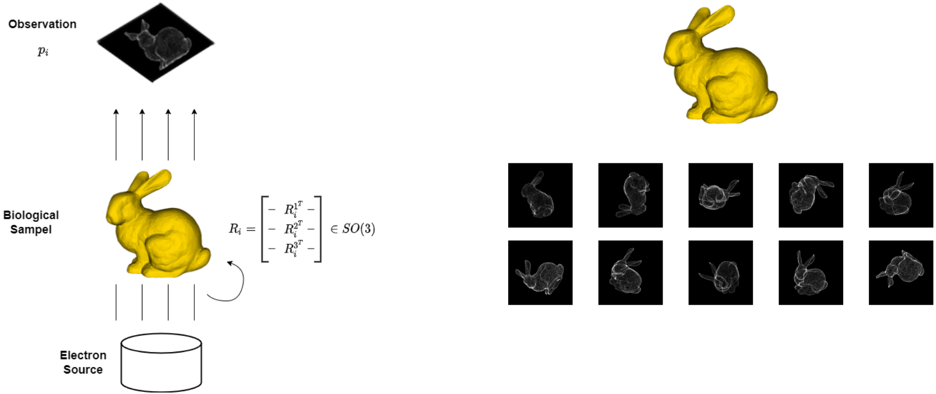
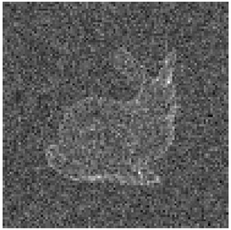


Figure: Cryo-EM overview

Cryo-EM challenges

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

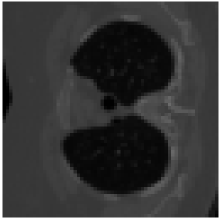
(a) Clean micrograph



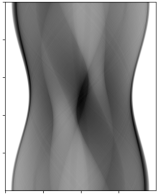
(b) Noisy micrograph

Computed Tomography (CT)

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



(a) Biological sampel



(b) clean Sinogram

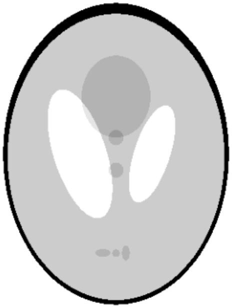
Observation

Observation

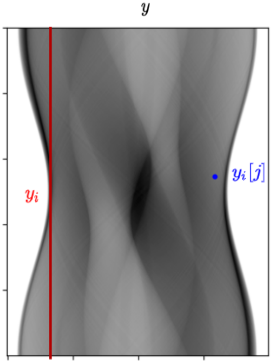
$$
\begin{aligned}
y &= p + \eta \\
y_i &= (A(x, \theta_i)) \\
y_i[j] &= p_i[j] + \eta_i[j] \quad \text{with } 1 \le i \le N, 1 \le j \le M
\end{aligned}
\tag{1}
$$

- y: noisy observation
- p: noiseless observation
- η: noise, assumed $\eta_i \sim \mathcal{N}(0, \sigma^2)$
- θ_i: observation angle
- N: number of observations
- M: observation dimension
- $A : L^2(\Omega) \to \mathbb{R}^M, x \mapsto A(x; \theta_i)$: a non-linear operator

Observation - Computed Tomography

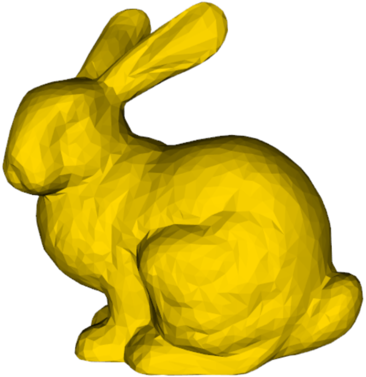


(a) Biological Sample



(b) CT Observation - sinogram

Observation - Cryo-EM



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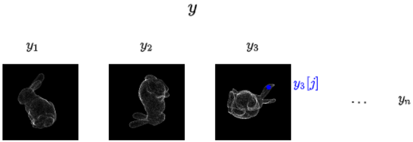


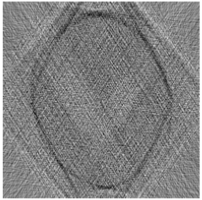
(b) Cryo-EM Observation - micrographs

Reconstruction

Reconstruction

$$\begin{aligned} Recon : \mathbb{R}^{M \times N} &\to \mathbb{R}^{M \times M} \\ y &\mapsto Recon(y; \theta) \end{aligned} \tag{2}$$

(a) Reconstruction clean: $Recon(p, \theta) \approx x$



(b) Reconstruction noisy: $Recon(p, \theta) \not\approx x$

Problem and Goal

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p not observable directly only y is observable.

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$$Recon\,(denoiser(y; \theta)) \approx x$$

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Graph - Definitions

Graph Definition

A graph is defined as $G = \langle V, E \rangle$, where V is a set of nodes and E is a set of edges.

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Nodes

$(n_1, n_2, \dots) \in \mathbb{R}^F$, with F as node feature dimensions.

Edges

Edges are defined as a set of tuples (i, j), where i and j determine the index of the nodes.

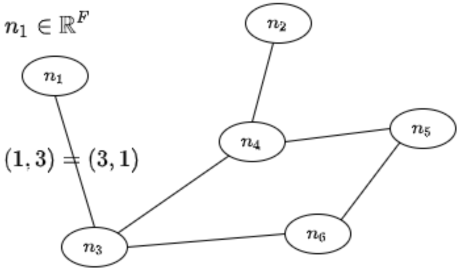

Figure: Sample graph

Graph - Definitions - Adjacency Matrix

Adjacency Matrix

The binary adjacency matrix of graph $G = \langle V, E \rangle$ is defined as:

$$A_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E \\ 0, & \text{otherwise} \end{cases} \tag{3}$$

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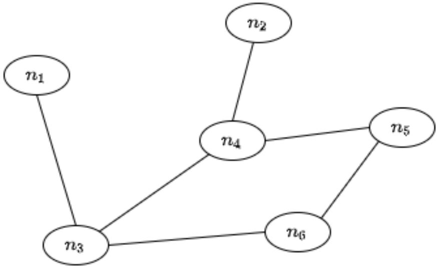

$$A = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}$$

Figure: Sample graph

Graph - Definitions - Degree

Degree of a node

The *degree* of a node is defined as the number of (incoming) edges.

Degree Matrix of Graph G

Is a diagonal matrix with degree of nodes as entries.

$$D_{ii} = degree(n_i)$$

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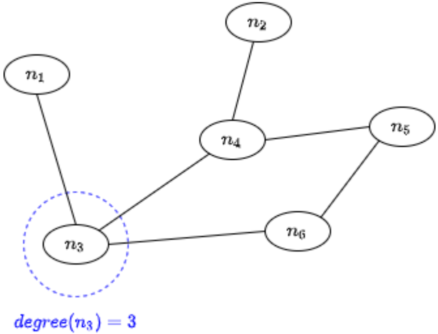

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Graph for Molecular Imaging Observation

- Nodes: Single observation y_i
- Edges: Use k-nearest neighbours (k-NN) to construct a graph
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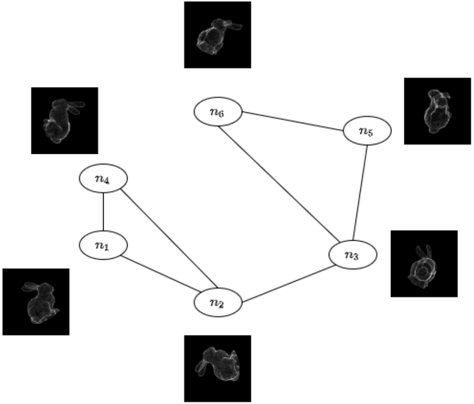


Figure: Sample graph for cryo-EM observation

Graph Laplacian (GL)

- What can we use this graph for?
- Coifman, Shkolnisky, et al. 2008 used it to approximate angles:

Low-dimensional Embedding

1. Construct a k-NN graph from observations.
2. Calculate $L = D - A$
3. Get 2nd and 3rd smallest eigenvalue with corresponding eigenvectors.

Lowdimensional Embedding

some notes and show clean embedding

Unknown angles

Show reconstruction with calculated angles

High-noise domain

Show graph Show embedding Show reconstruction

Graph Denoising

Graph denoising is the task, to estimate a denoised graph $\tilde{G}$ from a given noisy graph G_0, 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.

Traditional Denoising

BM3D Non-local means

Our Approach

BM3D Non-local means

Outline

Recap

Recap what we saw so far, define fixed angles

Big Picture

GAT-Denoiser : GNN Pipeline

Input Graph

how we defined our input graph.

Graph Attention Network - GAT

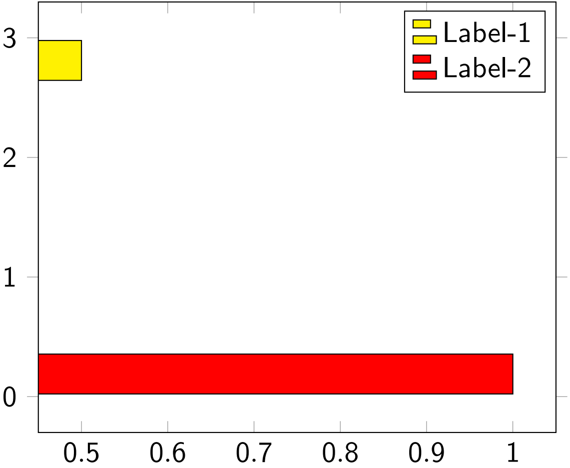
GAT, straight to the point

Expectation from components

expections from convolution,

Outline

Some result testing



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References

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