

Graph Denoising for Molecular Imaging

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Outline

- 1 Molecular Imaging Methods
- 2 Graphs & Manifolds
- 3 GAT-Denoiser
- 4 Results on LoDoPaB-CT dataset
- 5 Summary & Future Work
- 6 Questions

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Only single particle cryo-EM is considered.

Cryo-Electron Microscopy (Cryo-EM) - Illustration

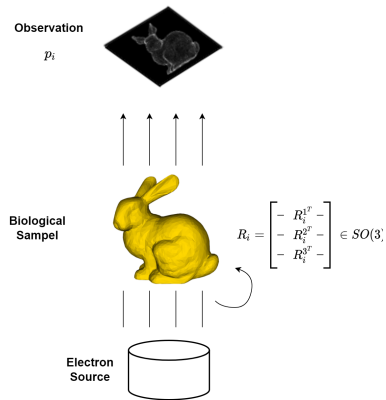


Figure: Cryo-EM overview

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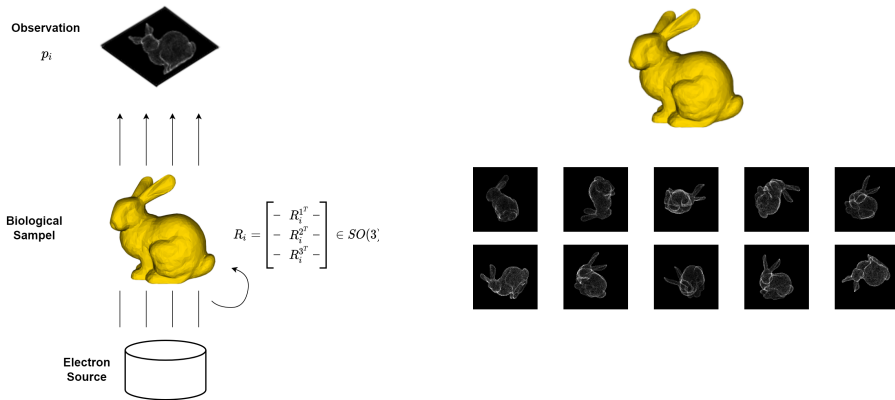


Figure: Cryo-EM overview

Cryo-Electron Microscopy (Cryo-EM) - Challenges

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



(a) Clean micrograph



(b) Noisy micrograph

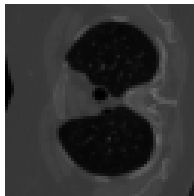
Computed Tomography (CT)

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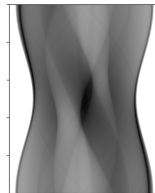
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(a) Biological sample



(b) Clean observation (sinogram)

Shared Observation Model

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Observation

$$y = p + \eta \quad (1)$$

- > y : noisy observation
- > p : noiseless observation
- > η : noise, assumed $\eta_i \sim \mathcal{N}(0, \sigma^2)$

Shared Observation Model

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

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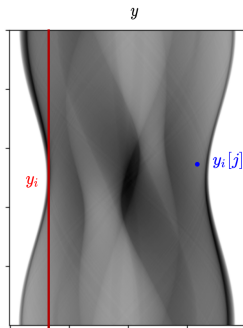
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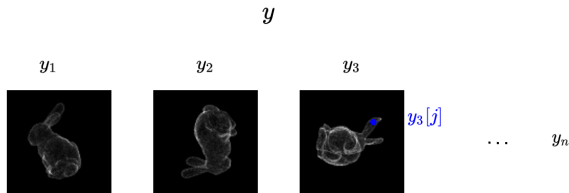
$$\begin{aligned} y &= p + \eta \\ y_i[j] &= p_i[j] + \eta_i[j] \quad \text{with } 1 \leq i \leq N, 1 \leq j \leq M \\ y_i &= A(x, \theta_i) + \eta_i \end{aligned} \tag{1}$$

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- > η : noise, assumed $\eta_i \sim \mathcal{N}(0, \sigma^2)$
- > x : biological sample
- > N : number of observations
- > M : observation dimension
- > $A : x \mapsto A(x; \theta_i) \in \mathbb{R}^M$: a non-linear operator
- > θ_i : observation angle

Observation - Illustration



(a) CT Observation - sinogram



(b) Cryo-EM Observation - micrographs

Reconstruction

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$$Recon : \mathbb{R}^{M \times N} \rightarrow \mathbb{R}^{M \times M} \quad y \mapsto Recon(y; \theta) \quad (2)$$

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- SNR is a measure, which compares the power of an input signal to the power of the undesired noise
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SNR is used as a metric for the quality of reconstructions.

Reconstruction - Computed Tomography

- Filter Backprojection (FBP)
 - Can be considered historical approach
 - Enables reconstruction for moderate noise

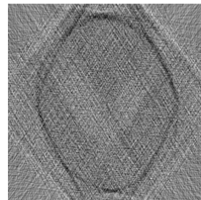
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(a) Reconstruction clean:

$$\text{Recon}(p, \theta) \approx x$$



(b) Reconstruction noisy

with SNR_y 0 dB:

$$\text{Recon}(y, \theta) \not\approx x$$

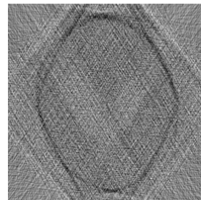
Reconstruction - Computed Tomography

- Filter Backprojection (FBP)
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- Neural Network Approaches
 - Today state-of-the art
 - Using result of FBP and further denoise
 - U-Net Ronneberger, Fischer, and Brox 2015



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p not observable directly only access to y .

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Goal

$$\text{denoiser} : y_i = (p_i + \eta) \mapsto p_i^* \approx p_i$$

$$\text{Recon}(\text{denoiser}(y; \theta)) \approx x$$

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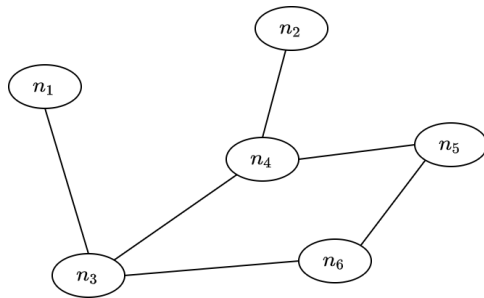


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Nodes

$(n_1, n_2, \dots) \in \mathbb{R}^F$, 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.

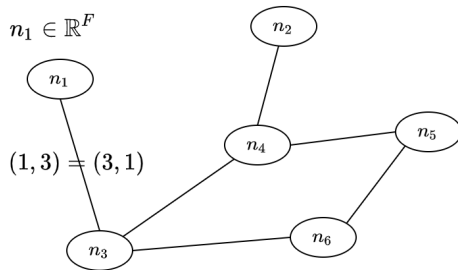


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Adjacency Matrix

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

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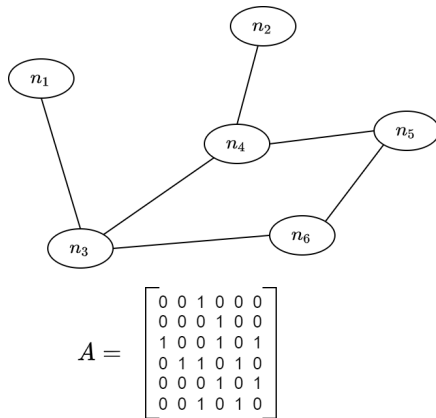


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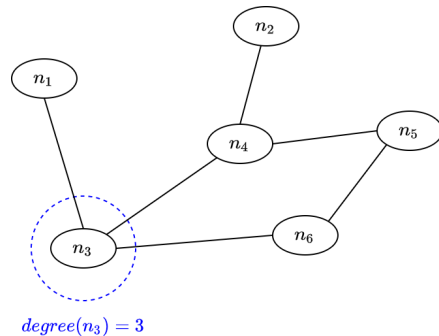


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Degree Matrix of Graph G

Is a diagonal matrix with degree of nodes as entries.

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

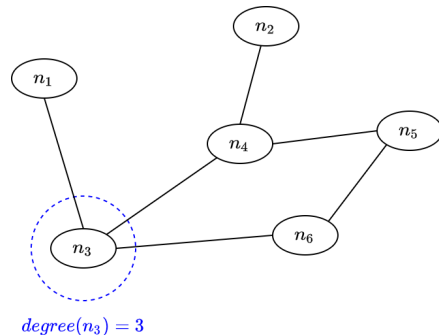


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Graph for Molecular Imaging Observation

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➤ Nodes: Single observation y_i

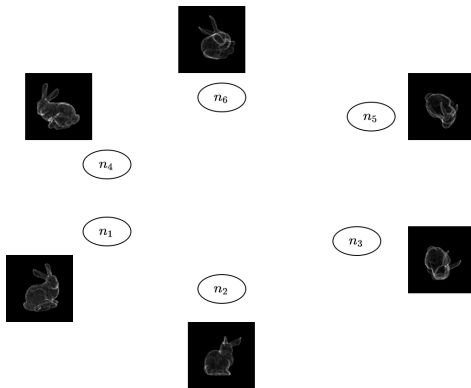


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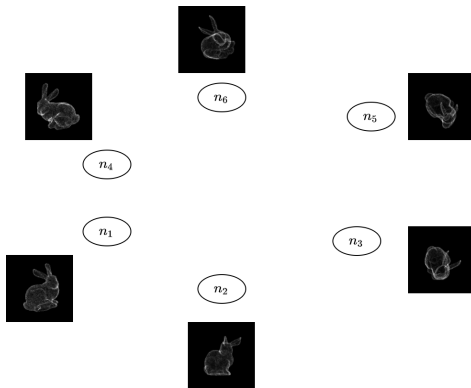


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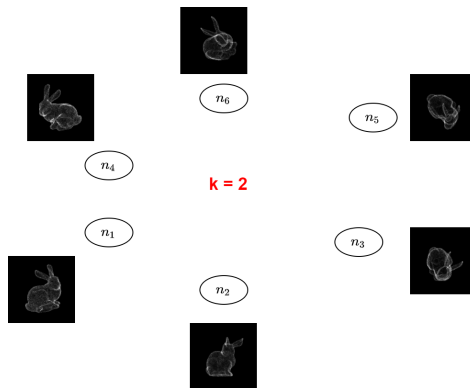


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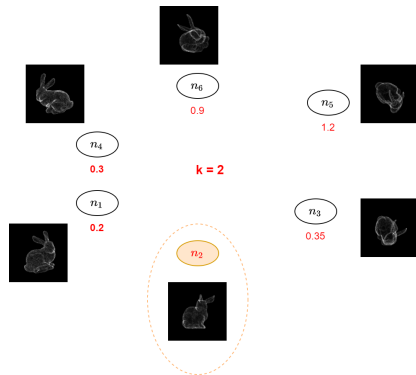


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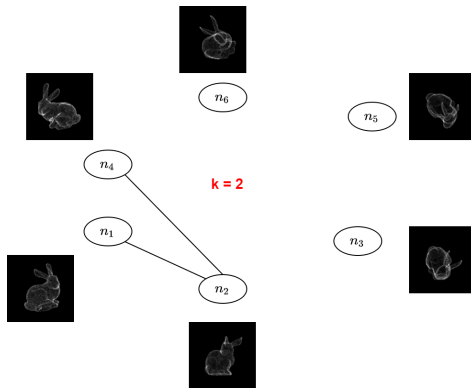


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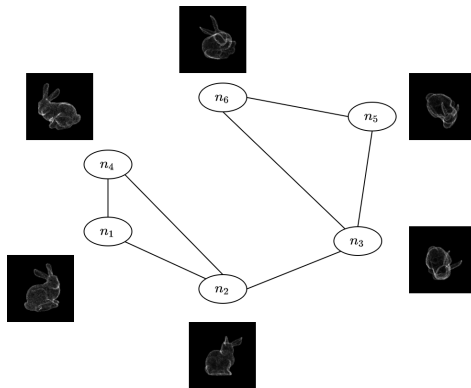


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Graph for Molecular Imaging Observation - Noise

What happens with our noisy observations?

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- > With noise, graph will capture neighborhood inaccurately.

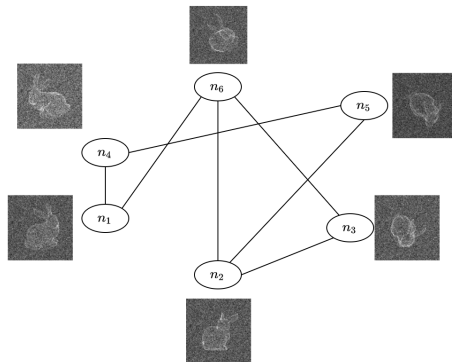


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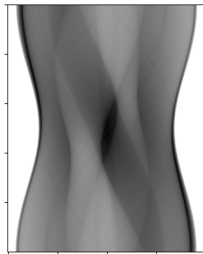
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Low-dimensional Embedding

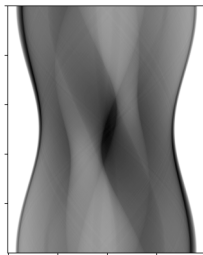
1. Construct a k-NN graph from observations.
2. Calculate $L = D - A$
3. Get 2nd and 3rd smallest eigenvalue with corresponding eigenvectors.

Low-dimensional Embedding for Computed Tomography

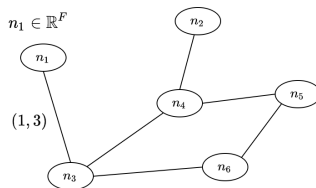


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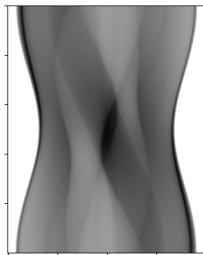


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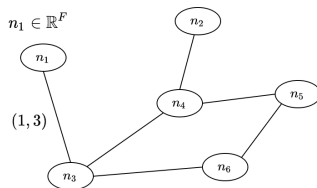


(b) Building k-NN graph with $k = 2$

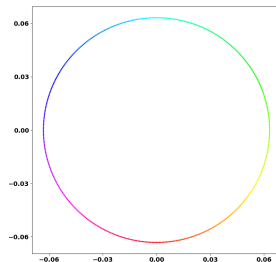
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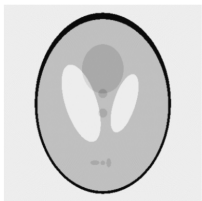
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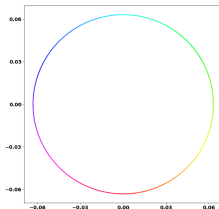
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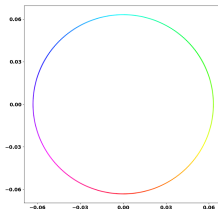
(b) GL-Embedding from $k = 2$

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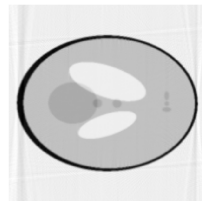
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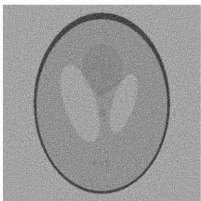
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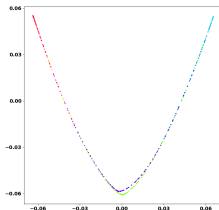
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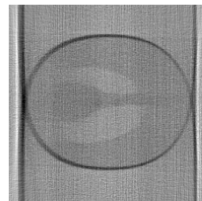
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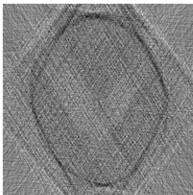
(b) GL-Embedding from $k = 6$ and $SNR_y : 10$ dB



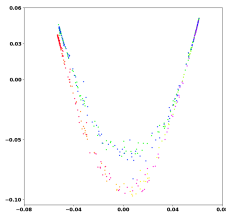
(c) Reconstruction unknown angles $SNR_y : 10$ dB

Computed Tomography with unknown angles

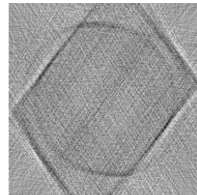
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Exploit graph as a data structure and the GL-Embedding

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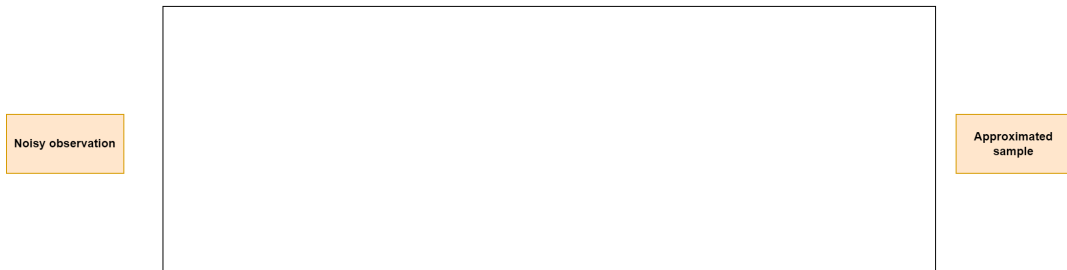
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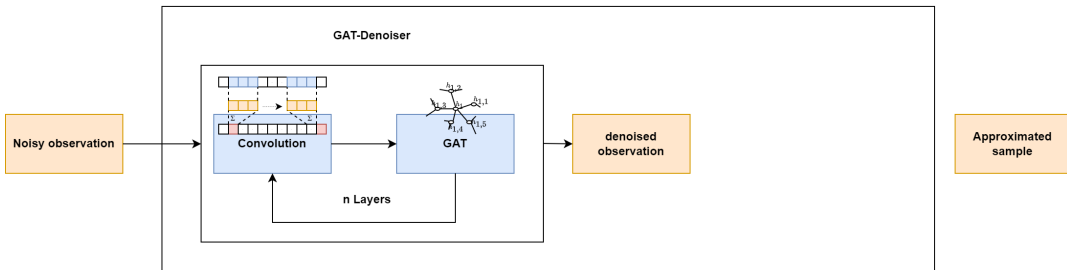
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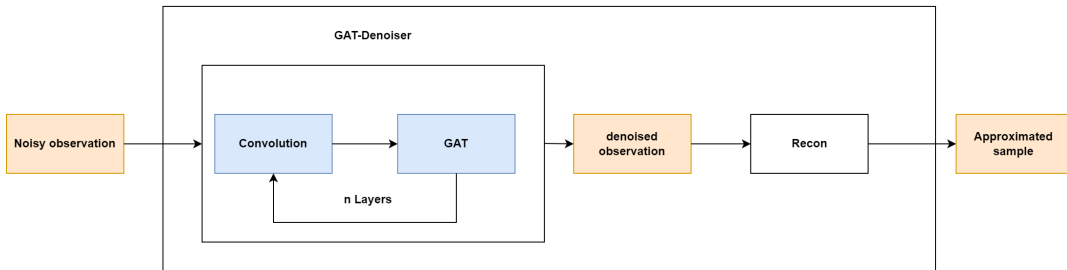
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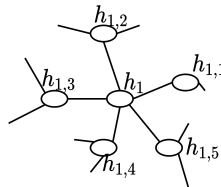
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 - › $\mathcal{L}_{\text{reconstruction}} = \| x - \text{Recon}(\text{GAT-Denoiser}(y)) \|_2^2$

Graph Attention Network - GAT

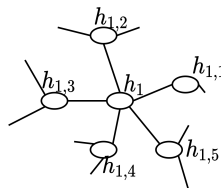
Graph Attention Network - GAT

- Extends Graph Convolution Network with attention (weights)
- Computes new node features
- Averages graph over neighborhood
- Multi-head available, motivated by Vaswani et al. 2017



Graph Attention Network - GAT

- Extends Graph Convolution Network with attention (weights)
- Computes new node features
- Averages graph over neighborhood
- Multi-head available, motivated by Vaswani et al. 2017
- σ : activation function (Exponential Linear Unit)
- W : learnable weight matrix
- α : normalized attention coefficients



$$h'_1 = \sigma \left(\sum_{i=1}^5 \alpha_i W h_{1,i} \right)$$

Input Graph

Input Graph

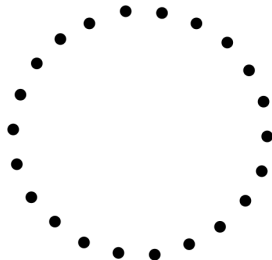
- › Exploit information from GL
 - › Low-dimensional embedding estimates angles
 - › Dominant information in data can be considered observation angles.

Input Graph

- › Exploit information from GL
 - › Low-dimensional embedding estimates angles
 - › Dominant information in data can be considered observation angles.
- › Construct graph from observation angles

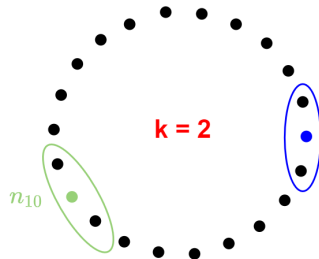
Input Graph

- › Exploit information from GL
 - › Low-dimensional embedding estimates angles
 - › Dominant information in data can be considered observation angles.
- › Construct graph from observation angles
 - › Map angles to unit-Circle or unit-sphere



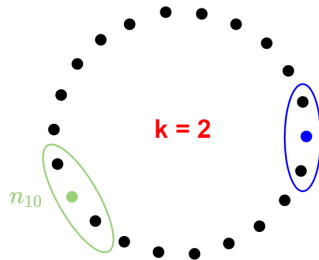
Input Graph

- Exploit information from GL
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Input Graph

- Exploit information from GL
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Observation angles θ are assumed to be equally spaced.

GAT-Denoiser Implementation for Computed Tomography

- › Use U-Net for reconstruction
- › During Trainig, U-Net might be trained jointly

Outline

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LoDoPaB-CT dataset

- Dataset for low-dose Computed Tomography
- 35'820 train samples
- 3'553 test samples
- BM3D as baseline algorithm
- Resolution 64×64

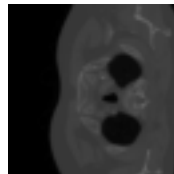
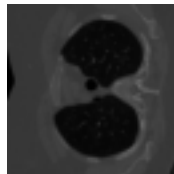
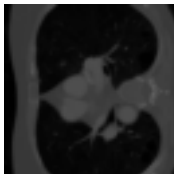


Figure: Some samples from the LoDoPaB-CT dataset.

Evaluation

> Small Scale Experiments

- > 1024 train samples
- > 100 test samples
- > 200 epochs

> Large Scale Experiments

- > Complete LoDoPaB-CT dataset
- > 20 - 40 epochs

Evaluation

> Small Scale Experiments

- > 1024 train samples
- > 100 test samples
- > 200 epochs
- > **Goal: Find most promising architecture**

> Large Scale Experiments

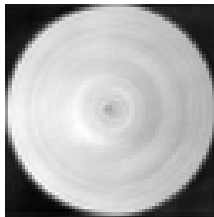
- > Complete LoDoPaB-CT dataset
- > 20 - 40 epochs
- > **Goal: Find best model**

Training

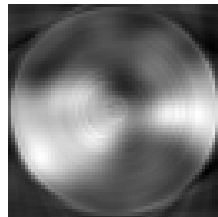
- U-Net used for reconstruction
 - Pre-trained with complete dataset and SNR_y in $[-10, 0]$ for 200 epochs
- Mini-batch gradient descent with batch size 64
- Adam optimizer
- Joint U-Net training possible

Small Scale Experiments - Overall Results

- Learning fails with random graph
- Learning succeeds with defined input graph



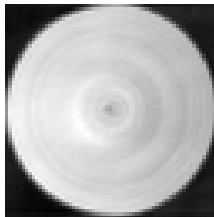
(a) Reconstruction with random input graph



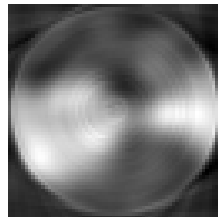
(b) Reconstruction with k-NN input graph $k = 10$

Small Scale Experiments - Overall Results

- Learning fails with random graph
- Learning succeeds with defined input graph
- Components contribute to success of GAT-Denoiser
- Best model with joint U-Net training

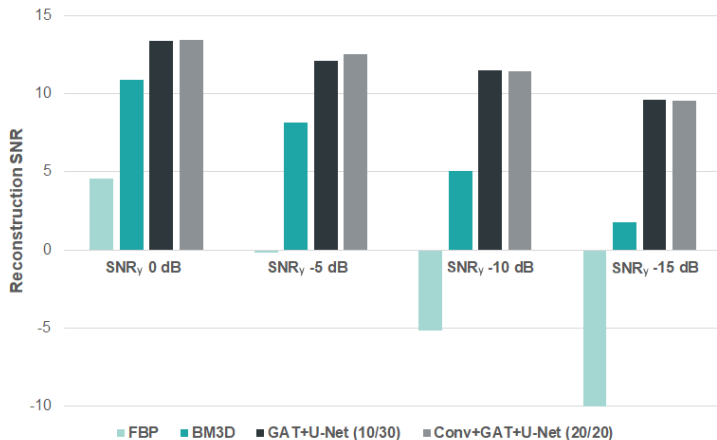


(a) Reconstruction with random input graph

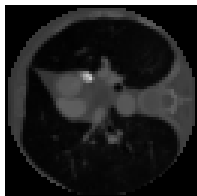


(b) Reconstruction with k-NN input graph $k = 10$

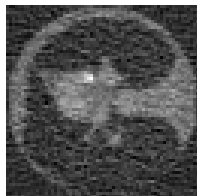
Large Scale Experiment - SNR Results



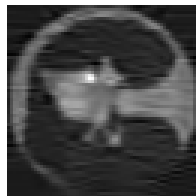
Large Scale Experiment - Visual Results - SNR_y 0 dB



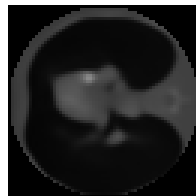
(a) Clean sample



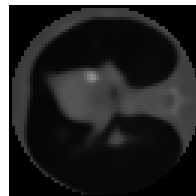
(b) FBP



(c) BM3D



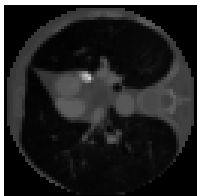
(d) $GAT+U-$
 $Net(10/30)$



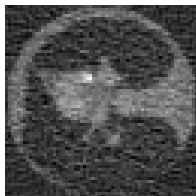
(e)
 $Conv+GAT+U-$
 $Net(20/20)$

Figure: Large Scale Experiment: Visual results for SNR_y 0 dB.

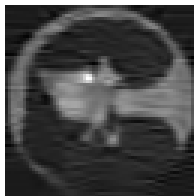
Large Scale Experiment - Visual Results - SNR_y 0 dB



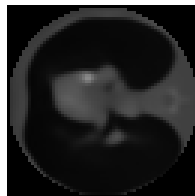
(a) Clean sample



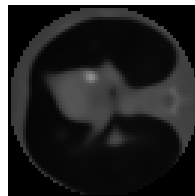
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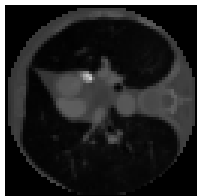


(e)
 $Conv+GAT+U-$
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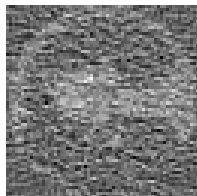
Figure: Large Scale Experiment: Visual results for SNR_y 0 dB.

GAT-Denoiser improves BM3D for SNR_y 0 dB by 27.6%.

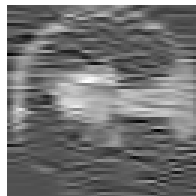
Large Scale Experiment - Visual Results - SNR_y -10 dB



(a) Clean sample



(b) FBP



(c) BM3D



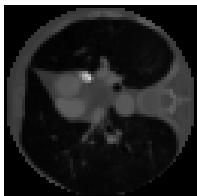
(d) $GAT+U-Net(10/30)$



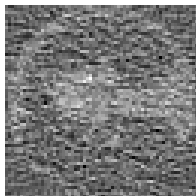
(e) $Conv+GAT+U-Net(20/20)$

Figure: Large Scale Experiment: Visual results for SNR_y -10 dB.

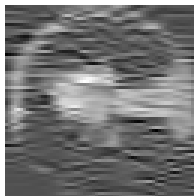
Large Scale Experiment - Visual Results - SNR_y -10 dB



(a) Clean sample



(b) FBP



(c) BM3D



(d) $GAT+U-Net(10/30)$

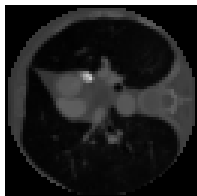


(e) $Conv+GAT+U-Net(20/20)$

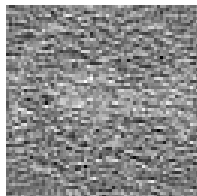
Figure: Large Scale Experiment: Visual results for SNR_y -10 dB.

GAT-Denoiser improves BM3D for SNR_y 0 dB by 126.0%.

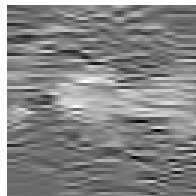
Large Scale Experiment - Visual Results - SNR_y -15 dB



(a) Clean sample



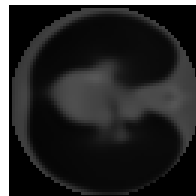
(b) FBP



(c) BM3D



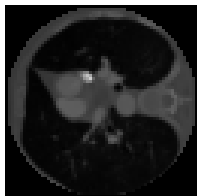
(d) *GAT+U-Net(10/30)*



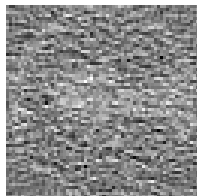
(e) *Conv+GAT+U-Net(20/20)*

Figure: Large Scale Experiment: Visual results for SNR_y -15 dB.

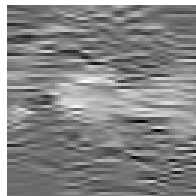
Large Scale Experiment - Visual Results - SNR_y -15 dB



(a) Clean sample



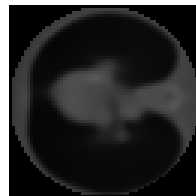
(b) FBP



(c) BM3D



(d) *GAT+U-Net(10/30)*



(e) *Conv+GAT+U-Net(20/20)*

Figure: Large Scale Experiment: Visual results for SNR_y -15 dB.

GAT-Denoiser improves BM3D for SNR_y 0 dB by 379.9%.

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Summary

- › GAT-Denoiser enables denoising of observations
 - › Convolution
 - › GAT
 - › End-To-End Learning
 - › Joint U-Net training boost performance

Summary

- › GAT-Denoiser enables denoising of observations
 - › Convolution
 - › GAT
 - › End-To-End Learning
 - › Joint U-Net training boost performance
- › Evaluated on LoDoPaB-CT dataset
 - › Outperformed baseline BM3D by up to 379.9 %

Future Work

- › Improve current GAT-Denoiser
- › Derive GAT-Denoiser for 3D
- › Make it work for unknown angles

Future Work

- › Improve current GAT-Denoiser
- › Derive GAT-Denoiser for 3D
- › Make it work for unknown angles
- › Cryo-EM
 - › Known angles
 - › Unknown angles
 - › Work with structural variety in observations

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Questions



References

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