

Reconstructing without Angles in Unknown-View Tomography

Zhizhen Jane Zhao

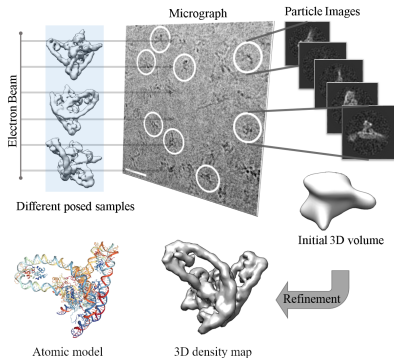
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ICERM Mathematics of 3D Reconstruction

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Introduction

- Scientific imaging is used to characterize physical, material, chemical, and biological processes.



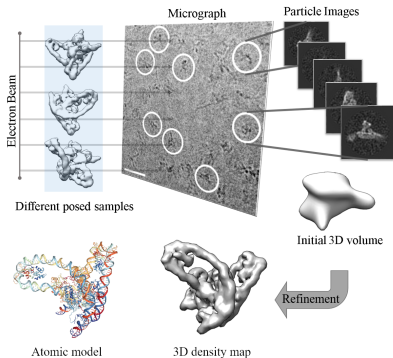
Cryo-electron microscopy single particle
analysis

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Imaging data challenges include

- Incomplete data
- measurement uncertainty (e.g., noise, unknown latent parameters)



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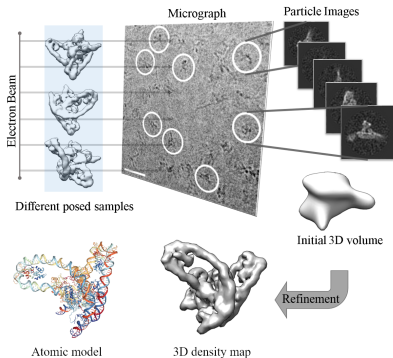
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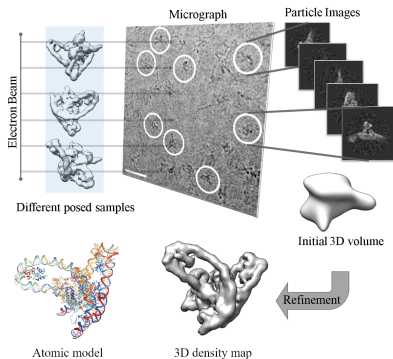
Here we focus on **tomography with unknown view angles**.



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Part I. Orthogonal matrix retrieval with spatial consensus

Joint work with Shuai Huang, Mona Zehni, and Ivan Dokmanic

Image formation model

- A simplified image formation model for a 3D electron density map ρ and $\omega_i \in \text{SO}(3)$:

$$\omega_i \circ \rho$$

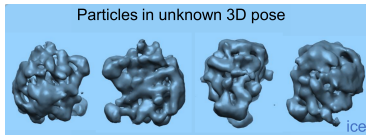
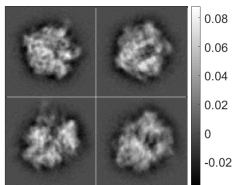
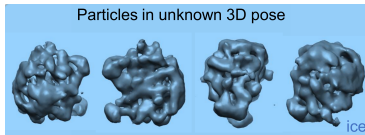


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$$I_i = P(\omega_i \circ \rho)$$



projections

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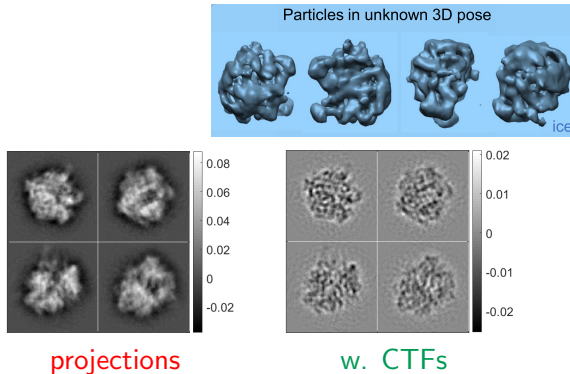
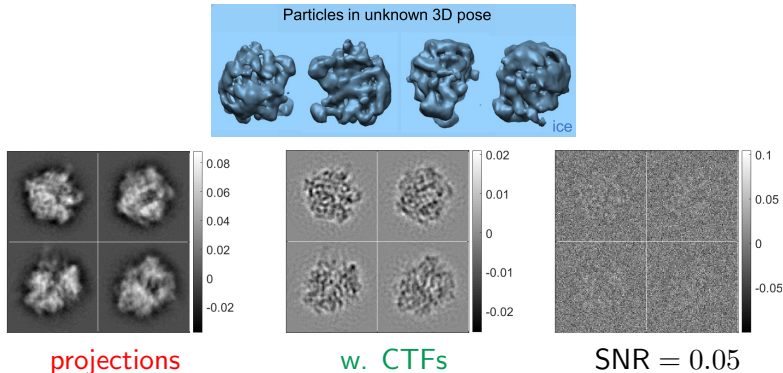


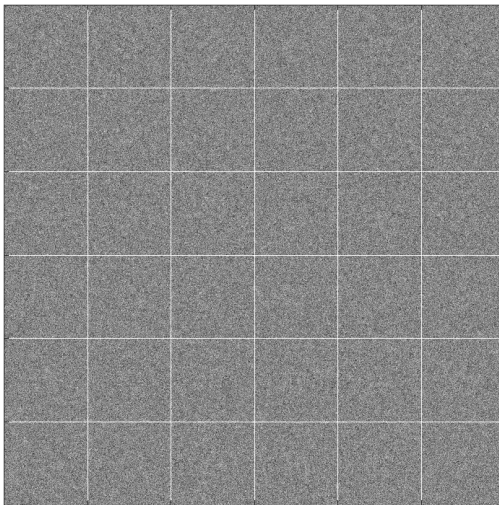
Image formation model

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$$I_i = H_i \star P(\omega_i \circ \rho) + \text{noise}$$



Noisy images



Typically contains over a million raw particle images

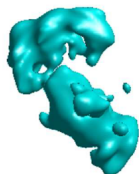
<https://www.ebi.ac.uk/pdbe/emdb/empiar/entry/10005/>



Traditional estimation approach

Alternate between estimating the particle orientation and reconstructing the 3D density

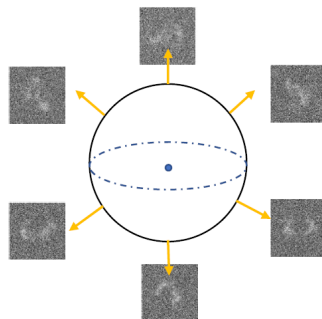
initialization



Orientation estimation



reconstruction



- Multiple passes over the whole data set

Method of moments

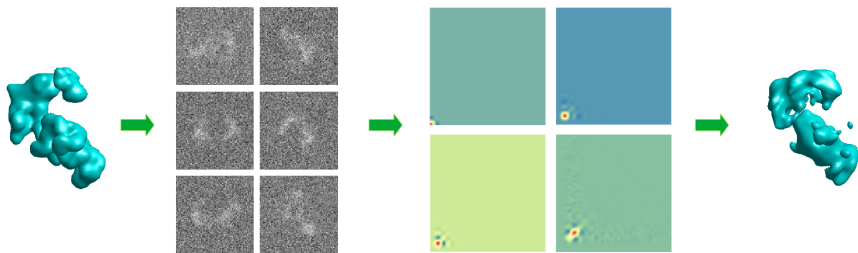
Reconstruct the 3D density via the method of moments

3D density map

Projections with
unknown orientations

Method-of-Moments features

Reconstruction



- Denoised moments can be obtained

Method of moments

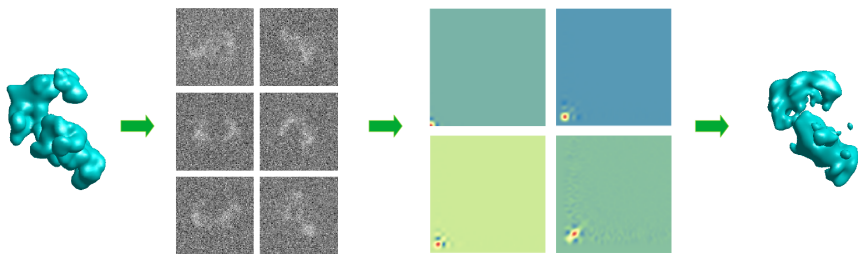
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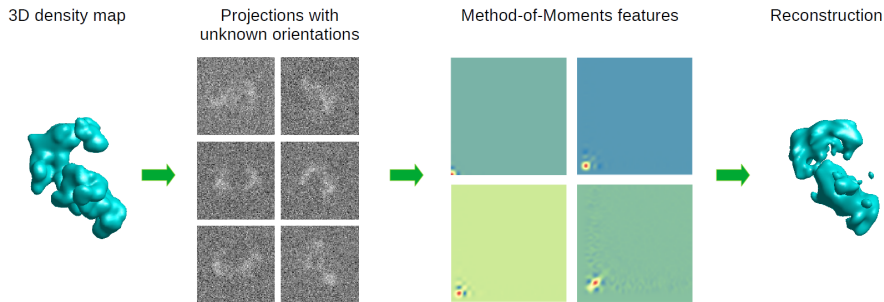
Reconstruction



- Denoised moments can be obtained
- Only go through the images once to extract features
- Bypass the orientation estimation

Method of moments

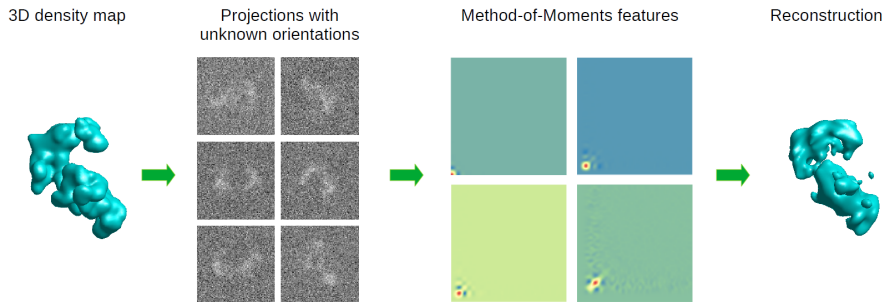
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Method of moments

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- Denoised moments can be obtained
- Only go through the images once to extract features
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- The sample complexity scales as σ^{2m} for the estimation of m^{th} order moments
- Some assumptions: centered images, distribution of the orientations is uniform over $\text{SO}(3)$

Projection-slice theorem

- Let $\mathbf{R}_i$ be the rotation matrix corresponding to ω_i , for clean measurement data, we have

$$\hat{I}_i(k_x, k_y) = \hat{\rho}(\mathbf{R}_i^T [k_x \ k_y \ 0]^T)$$

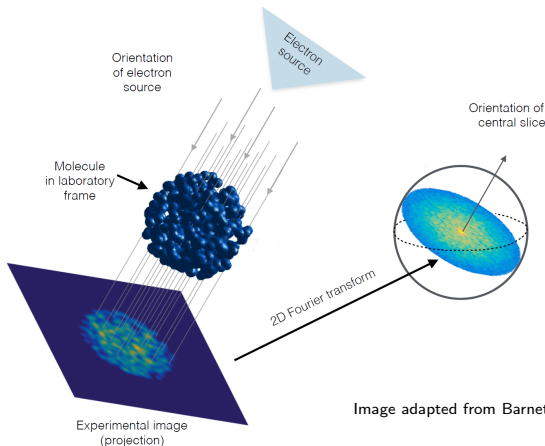


Image adapted from Barnett et al. SIIMS, 2017

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- Spherical harmonic expansion:

$$\hat{\rho}(\mathbf{k}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l A_{lm}(\mathbf{k}) \cdot Y_{lm}(\theta_{\mathbf{k}}, \varphi_{\mathbf{k}}),$$

$A_{lm}(\mathbf{k})$ is the real spherical harmonic expansion coefficients.

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- In terms of the spherical expansion coefficients,

$$\hat{I}_i(k_x, k_y) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{m'=-l}^l A_{lm}(\mathbf{k}) \cdot Y_{lm'}\left(\frac{\pi}{2}, \varphi_{\mathbf{k}}\right) \cdot D_{mm'}^l(\omega_i),$$

where D^l is the Wigner D -matrix.

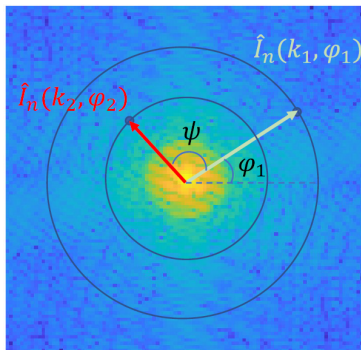
Kam's autocorrelation analysis

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$$C_N(k_1, k_2, \psi) = \frac{1}{N} \sum_{n=1}^N \frac{1}{2\pi} \int_0^{2\pi} \hat{I}_n(k_1, \varphi_1) \cdot \hat{I}_n^*(k_2, \varphi_1 + \psi) d\varphi_1$$



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- For clean images,

$$C_N(k_1, k_2, \psi) \xrightarrow{N \rightarrow \infty} \underbrace{\frac{1}{4\pi} \sum_{l=0}^{\infty} P_l(\cos \psi) \sum_{m=-l}^l A_{lm}(k_1) \cdot A_{lm}^*(k_2)}_{=: C(k_1, k_2, \psi)},$$

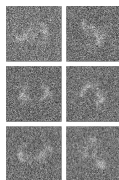
where $P_l(\cdot)$ is the Legendre polynomial of degree l , and $C(k_1, k_2, \psi)$ is the asymptotic noiseless autocorrelation function of the Fourier transform $\hat{\rho}(\mathbf{k})$ in the frequency domain over the rotation group $SO(3)$.

Kam's autocorrelation analysis

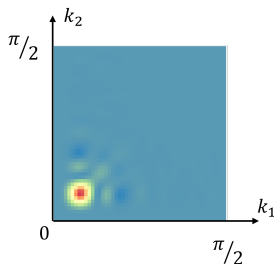
- Kam further computed the contribution of the subspace of all spherical harmonics with degree l , using orthogonality of Legendre polynomials,

$$\begin{aligned} C_l(k_1, k_2) &= 2\pi(2l+1) \int_0^\pi C(k_1, k_2, \psi) \cdot P_l(\cos \psi) \cdot \sin \psi \, d\psi \\ &= \sum_{m=-l}^l A_{lm}(k_1) \cdot A_{lm}^*(k_2), \quad l = 0, 1, \dots, L \end{aligned}$$

Projections with
unknown orientations



Feature matrix C_l

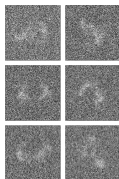


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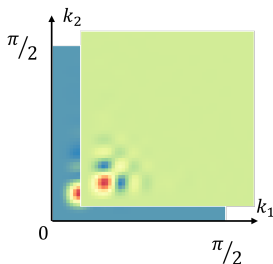
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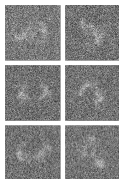


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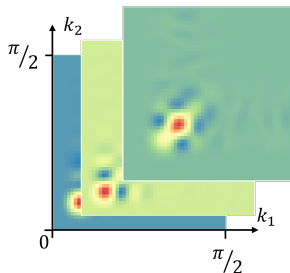
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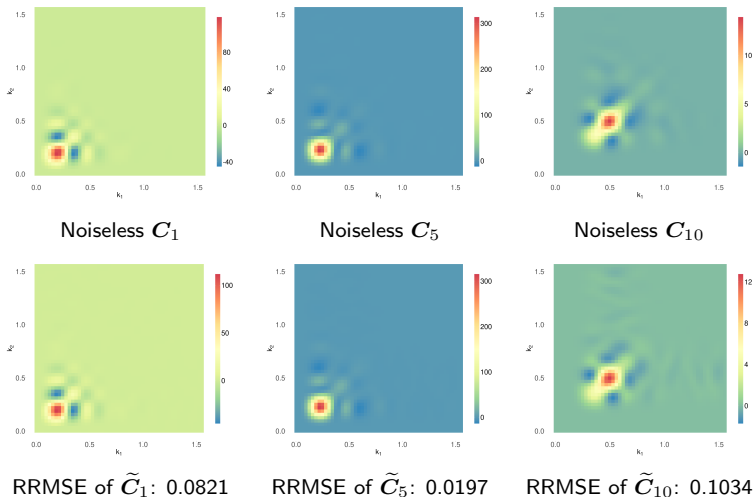
Projections with
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Feature matrix C_l



Estimated autocorrelation features



Fourier autocorrelation feature $\tilde{C}_l$ is extracted from $N = 10^4$ projection images with SNR=0.1.

Zhao et al., Fast steerable principal component analysis, IEEE TCI, 2016.

Bhamre et al., Denoising and covariance estimation of single particle cryo-EM Images, JSB, 2016

Navigation icons: back, forward, search, etc.

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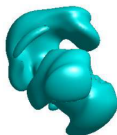
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- Truncated reconstruction:

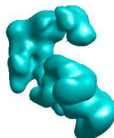
$L = 6$



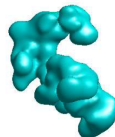
$L = 10$



$L = 16$



$L = 20$



Orthogonal matrix retrieval

- We have for any orthogonal $\mathbf{O}_l$ of size $(2l + 1) \times (2l + 1)$ that

$$\mathbf{C}_l = \mathbf{A}_l \mathbf{O}_l^T (\mathbf{A}_l \mathbf{O}_l^T)^* = \mathbf{F}_l \mathbf{F}_l^* .$$

*T. Bhamre, T. Zhang, and A. Singer, Orthogonal matrix retrieval in cryo-electron microscopy, ISBI, 2015

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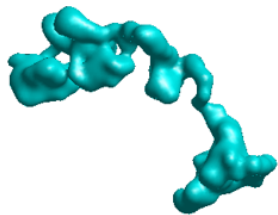
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- For a pair of images I_1 and I_2 , we have $\rho_2 = \omega \circ \rho_1$, with $\omega \in \text{SO}(3)$. Optimize over $\{\mathbf{O}_l\}_{l=1}^L$ and ω .

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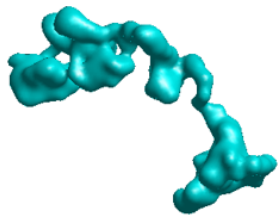
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Challenges in OMR

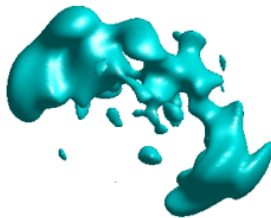


Ground truth

Challenges in OMR

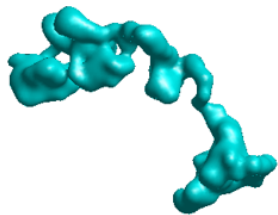


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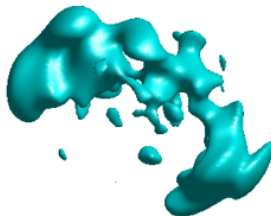


Clean reconstruction

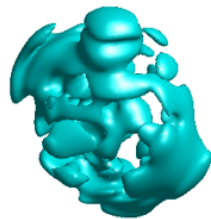
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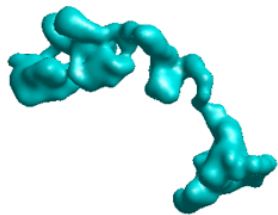


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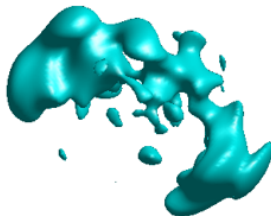


Noisy reconstruction

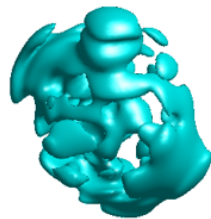
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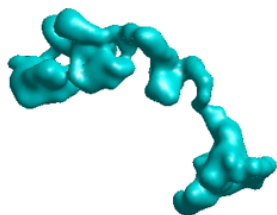
Clean reconstruction



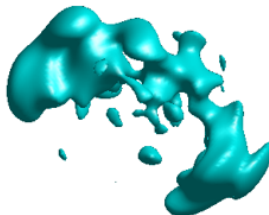
Noisy reconstruction

- Previous approach focuses mainly on the recovery of O_l

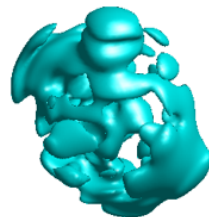
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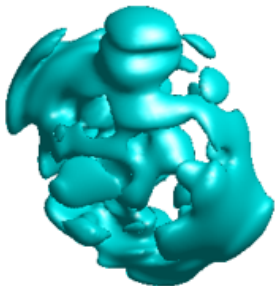
Clean reconstruction



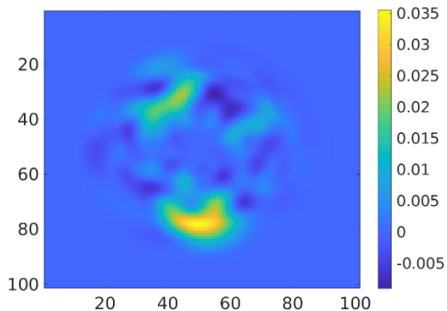
Noisy reconstruction

- Previous approach focuses mainly on the recovery of O_l
- Not robust enough in the noisy case (SNR= 0.1)

Challenges with OMR

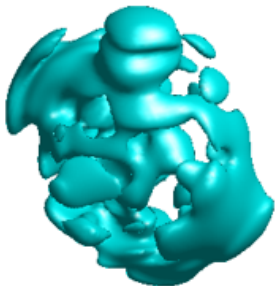


Noisy reconstruction

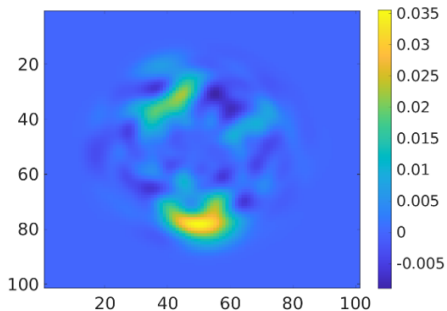


A 2D slice

Challenges with OMR



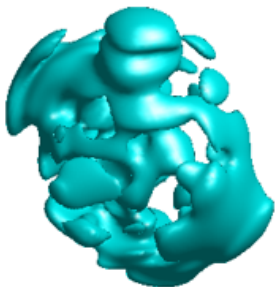
Noisy reconstruction



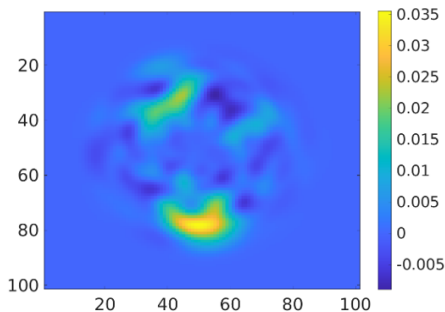
A 2D slice

- How to enforce that the reconstructed density map is non-negative

Challenges with OMR



Noisy reconstruction



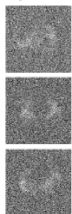
A 2D slice

- How to enforce that the reconstructed density map is non-negative
- How to improve the reconstruction quality from the noisy measurements

Spatial constraints on the density map

- Non-negativity and total mass constraint

random
projections



⋮

average
projection



total mass

$$W_\rho = \|\rho\|_1$$

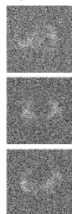
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$$\|\rho\|_1 = \sum_{d=1}^D |\rho_d| = W_\rho$$

Spatial constraints on the density map

- Non-negativity and total mass constraint

random
projections



⋮

average
projection



total mass

$$W_\rho = \|\rho\|_1$$

$$0 \leq \rho_d < W_\rho, \quad d = 1, \dots, D$$

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- Reference projection (randomly chosen): $P_\rho(x, y) = I(x, y)$

Spatial autocorrelation features

- The density map has the following real spherical harmonic expansion,

$$\rho(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l B_{lm}(r) \cdot Y_{lm}(\theta_{\mathbf{r}}, \varphi_{\mathbf{r}}).$$

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$$C_l(k_1, k_2) = 8\pi^2 \int_0^{\infty} \left(\int_0^{\infty} E_l(r_1, r_2) \cdot j_l(k_1 r_1) r_1^2 dr_1 \right) \cdot j_l(k_2 r_2) r_2^2 dr_2.$$

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- Use the quadrature points and weights according to Gauss-Legendre Quadrature rule, we express the relations in the matrix form,

$$\mathbf{A}_l = \mathbf{Q}_l^* \mathbf{B}_l, \quad \mathbf{F}_l \mathbf{O}_l = \mathbf{Q}_l^* \mathbf{B}_l(\rho), \quad \mathbf{B}_l(\rho) \text{ is linear in } \rho$$

Spatial radial features

- We average $\hat{I}_n(\mathbf{k})$ over all directions of $\mathbf{k}$ with the same norm k :

$$M_N(k) = \frac{1}{N} \sum_{n=1}^N \frac{1}{2\pi} \int_0^{2\pi} \hat{I}_n(\mathbf{k}) d\varphi$$

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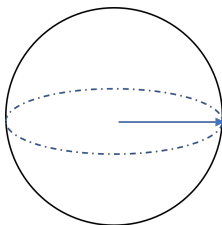
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$$W(r) = \frac{2r}{\pi} \int_0^\infty k \cdot \mathbf{M}(\mathbf{k}) \cdot \sin(kr) dk = \iiint \rho(\tilde{\mathbf{r}}) \cdot \delta(\tilde{r} - r) d\tilde{\mathbf{r}}.$$



Integration of ρ on a sphere

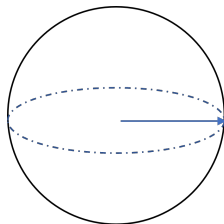
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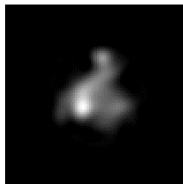
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Integration of ρ on a sphere



Denoised reference image

Orthogonal matrix retrieval with spatial consensus

We formulate the following nonconvex problem to recover the density in the spatial domain:

$$\underset{\rho, \{\mathbf{O}_l\}_{l=0}^L}{\text{minimize}} \quad f(\rho, \mathbf{O}_l) := \sum_{l=0}^L \|\mathbf{F}_l \mathbf{O}_l - \mathbf{Q}_l^* \mathbf{B}_l(\rho)\|_2^2$$

autocorrelation features

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Alternating minimization

Given an initialization ρ_0 , we use the following alternating minimization approach:

- **(O-update).** Fix ρ , and update $\{\mathbf{O}_l\}_l$ with respect to ρ :

$$\begin{aligned} \underset{\{\mathbf{O}_l\}_{l=0}^L}{\text{minimize}} \quad & f_1(\mathbf{O}_l) := \sum_{l=0}^L \|\mathbf{F}_l \mathbf{O}_l - \mathbf{Q}_l^* \mathbf{B}_l(\rho)\|_2^2 \\ \text{subject to} \quad & \mathbf{O}_l^T \mathbf{O}_l = \mathbf{O}_l \mathbf{O}_l^T = \mathbf{I}, \quad l \in \{0, \dots, L\}. \end{aligned}$$

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Closed-form solutions for the orthogonal matrices $\{\mathbf{O}_l\}_l$ are given by

$$\mathbf{O}_l = \mathbf{V}_l \mathbf{U}_l^T,$$

where $\mathbf{V}_l$ and $\mathbf{U}_l$ are obtained from the singular value decomposition (SVD) of $\mathbf{B}_l^T(\rho) \mathbf{Q}_l \mathbf{F}_l$

Alternating minimization

- (**ρ -update**). Fix $\{\mathbf{O}_l\}_l$, and estimate ρ with respect to $\{\mathbf{O}_l\}_l$:

$$\begin{aligned} \underset{\rho}{\text{minimize}} \quad & f_2(\rho) := \sum_{l=0}^L \|\mathbf{F}_l \mathbf{O}_l - \mathbf{Q}_l^* \mathbf{B}_l(\rho)\|_2^2 \\ & + \lambda \cdot \sum_{v=1}^V \left(\mathbf{g}_v^T \rho - W_v \right)^2 \\ & + \xi \cdot \sum_{x,y} \left(P_\rho(x,y) - \bar{I}(x,y) \right)^2, \\ \text{subject to} \quad & 0 \leq \rho_d \leq W_\rho, \\ & \sum_{d=1}^D \rho_d = W_\rho. \end{aligned}$$

- A convex problem which can be solved using projected gradient descent (PGD).

An Initialization

- Compute an initialization ρ_0 by solving the following problem:

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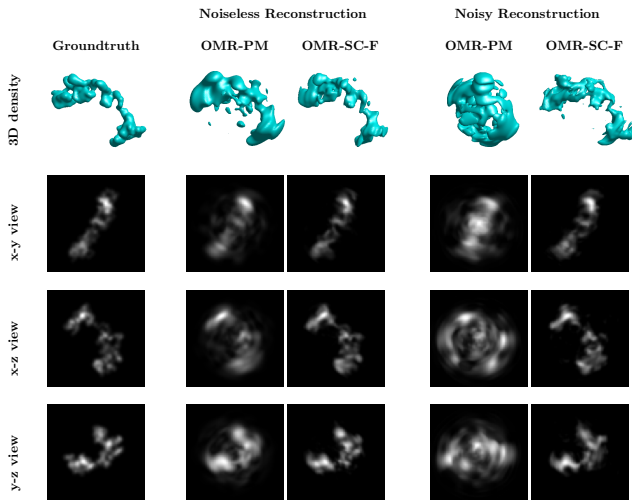
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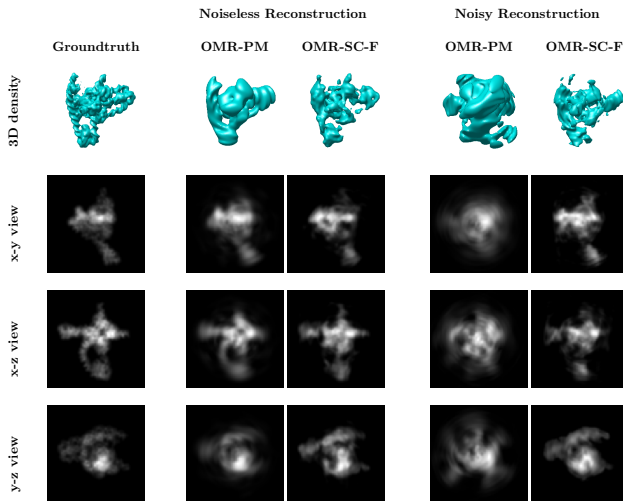
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- We use projected gradient descent initialized at $\mathbf{0}$ that favors the minimum l_2 -norm solution.

Reconstructions

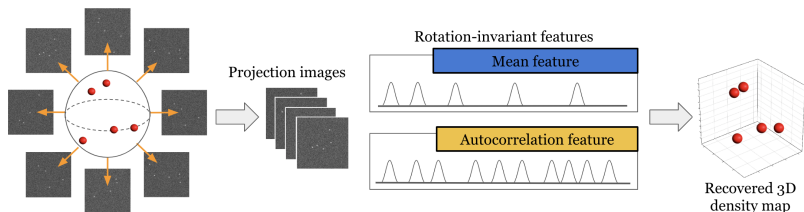


Reconstructions



Holliday junction complex (HJC): reconstructions using the OMR-PM and OMR-SC-F approaches in the noiseless case and the noisy case (SNR=0.1).

Sparsity

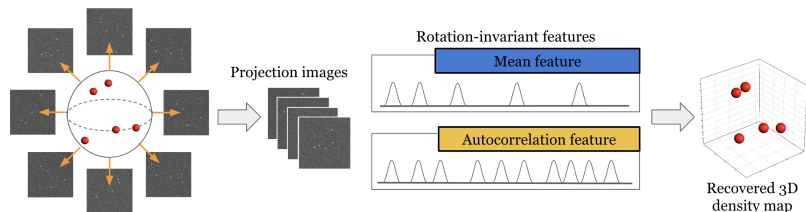


- A subset of the autocorrelation features can recover the density modeled as a mixture of Gaussians ^{*}.

^{*}M. Zehni et al. "3D unknown view tomography via rotation invariants" *ICASSP*, 2020.

[†]T. Bendory et al. "Autocorrelation analysis for cryo-EM with sparsity constraints: Improved sample complexity and projection-based algorithms" *PNAS*, 2023.

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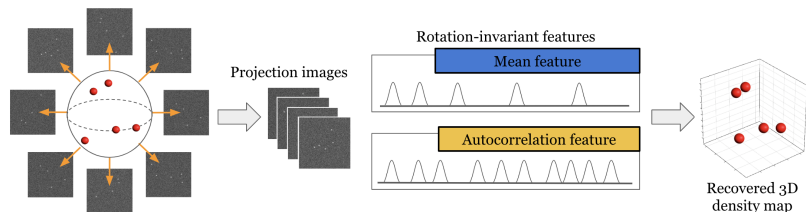


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- Bendory et al.[†] proved that 3D density maps modeled as sums of Gaussians (with some assumptions) are uniquely determined by the second-order autocorrelation of their projection images.
- The sample complexity is proportional to σ^4 .

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Summary and discussions

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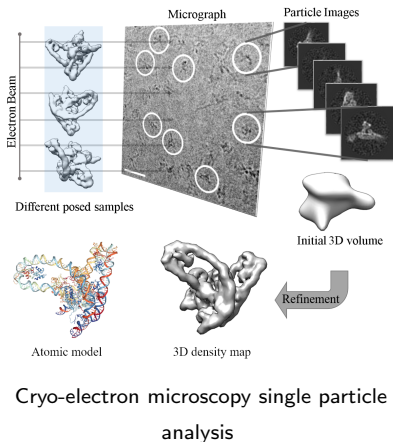
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Summary and discussions

- Using Kam's autocorrelation analysis with non-negative constraint on the voxel values, we are able to recover the 3D volumes without estimating the individual orientation
- How to incorporate more prior information about the density maps
- Require more thorough theoretical analysis on the uniqueness guarantee given certain types of spatial constraints or prior information
- Need to understand the landscape of the associated optimization problems

Introduction

- Scientific imaging is used to characterize physical, material, chemical, and biological processes.



Imaging data challenges include

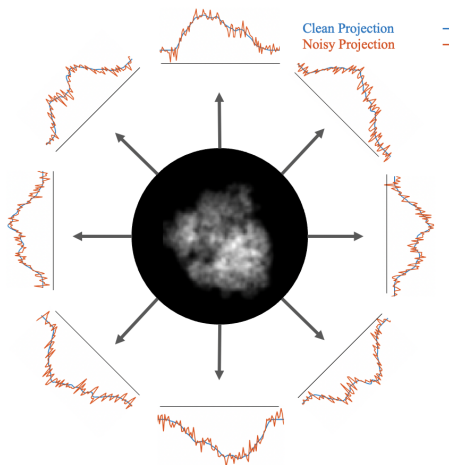
- Incomplete data
- measurement uncertainty (e.g., noise, unknown latent parameters)

Here we focus on **tomography with unknown view angles**.

Part II. Combine distribution matching and physics-based imaging process

Joint work with Mona Zehni

2D Tomography with unknown view angles



Noisy measurements:

$$\zeta_\ell = \mathcal{P}_{\theta_\ell} I + \varepsilon_\ell$$

$$\theta_\ell \sim p(\theta)$$

Goal

Recover I and p given
unordered $\{\zeta_\ell\}_{\ell=1}^L$.

2D tomography with unknown view angles

- Viewing angle estimation (angle recovery problem¹², graph Laplacian tomography³⁴, Moment-based angular difference estimates (MADE)⁵) and tomographic reconstruction
- Maximum likelihood estimation or maximum a posteriori estimation using expectation-maximization algorithm.
- Generative adversarial learning based approach⁶⁷

¹ Basu and Bresler, Uniqueness of tomography with unknown view angles, *IEEE TIP*, 2000

² Basu and Bresler, Feasibility of tomography with unknown view angles, *IEEE TIP*, 2000

³ Coifman et al., Graph Laplacian Tomography From Unknown Random Projections, *IEEE TIP*, 2008

⁴ Singer and Wu, Two-dimensional tomography from noisy projections taken at unknown random directions, *SIIMS*, 2013

⁵ Phan et al., Moment-Based Angular Difference Estimation Between Two Tomographic Projections in 2D and 3D, *J Math Imaging Vis* 2016.

⁶ Gupta et al. CryoGAN: A New Reconstruction Paradigm for Single-particle Cryo-EM Via Deep Adversarial Learning, *IEEE TCI*, 2021.

⁷ Zehni and Zhao, UVTomo-GAN: An adversarial learning based approach for unknown view X-ray tomographic reconstruction, *ISBI*, 2021

Viewing angle estimation

Graph Laplacian tomography:

- Apply PCA and Wiener filtering to denoise the projections.
- Compute pairwise distance between the denoised projections
$$d_{ij} = \|\zeta_i - \zeta_j\|_2.$$
- Construct k nearest neighbor graph followed by graph denoising.
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Main Challenge: The projection moment-based features used in the MADE are sensitive to noise.

Bypassing individual view angle estimation?

- **Question:** Can we achieve good image reconstruction without the estimation of individual view angles?

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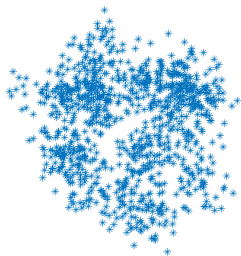
Bypassing individual view angle estimation?

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- **Challenge:** recover both the image and the viewing angle distribution simultaneously.

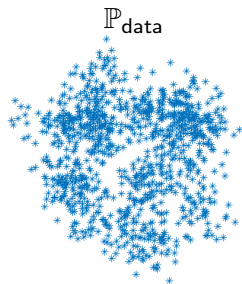
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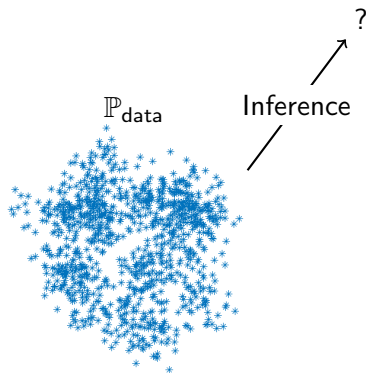
Reconstruction based on distribution matching



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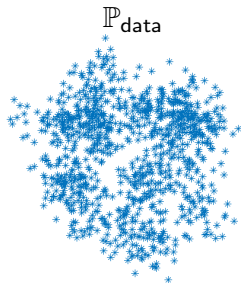


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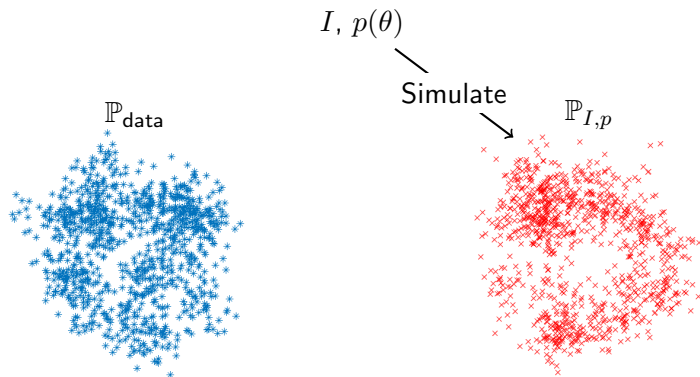


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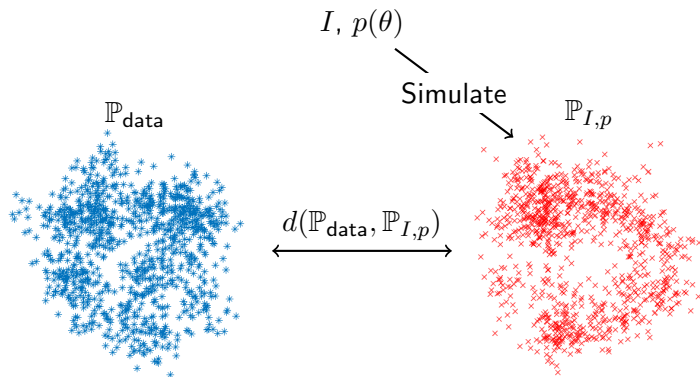
$$I, p(\theta)$$



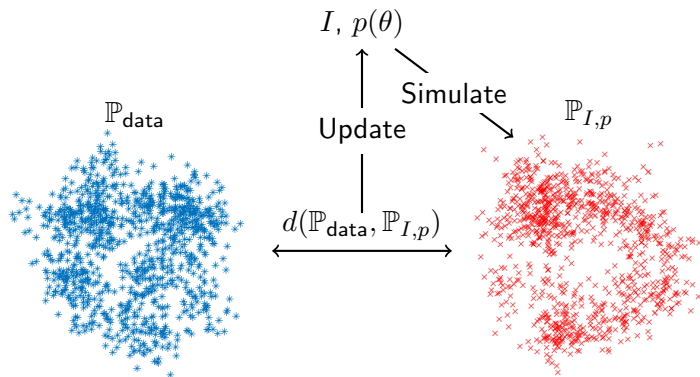
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Reconstruction based on distribution matching



Statistical inference is performed by minimizing, over the parameter space, the distance / divergence between model distribution and the empirical distribution of the data.

Comparing probability distributions

- KL divergence, Jensen-Shannon divergence, total variation, MMD...

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- The Earth-Mover's distance or Wasserstein-1 distance using Kantorovich-Rubinstein duality

$$W(\mathbb{P}_{\text{data}}, \mathbb{P}_{I,p}) = \sup_{\|f\|_L \leq 1} \mathbb{E}_{x \sim \mathbb{P}_{\text{data}}} [f(x)] - \mathbb{E}_{x \sim \mathbb{P}_{I,p}} [f(x)].$$

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- The Earth-Mover's distance or Wasserstein-1 distance

$$W(\mathbb{P}_{\text{data}}, \mathbb{P}_{I,p}) = \inf_{\gamma \in \Pi(\mathbb{P}_{\text{data}}, \mathbb{P}_{I,p})} \mathbb{E}_{(x,y) \sim \gamma} [\|x - y\|].$$

- The Earth-Mover's distance or Wasserstein-1 distance using Kantorovich-Rubinstein duality

$$W(\mathbb{P}_{\text{data}}, \mathbb{P}_{I,p}) = \sup_{\|f\|_L \leq 1} \mathbb{E}_{x \sim \mathbb{P}_{\text{data}}} [f(x)] - \mathbb{E}_{x \sim \mathbb{P}_{I,p}} [f(x)].$$

- Earth-Mover's distance has nicer properties than Jensen-Shannon divergence or KL divergence in learning distributions, specifically for distributions supported on lower dimensional manifolds.

Image representation

We use the Hartley transform of the images, which is a real representation closely related to Fourier transform and defined as:

$$\tilde{I} = \mathcal{H}(I) = \text{real}\{\mathcal{F}(I)\} - \text{imag}\{\mathcal{F}(I)\},$$

- Projection slice theorem in Hartley domain: $\tilde{\zeta}_\ell(\xi) = \tilde{I}(\xi, \theta_\ell)$

¹A. Klug and R. Crowther, "Three-dimensional image reconstruction from the viewpoint of information theory," *Nature*, vol. 238, no. 5365, pp. 435–440, 1972.

²Zhao and Singer, "Fourier–Bessel rotational invariant eigenimages", *JOSA A*, vol. 30, pp. 871–877, 2013

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$$\tilde{I}(\xi, \theta) \approx \sum_{k=-k_{\max}}^{k_{\max}} \sum_{q=1}^{p_k} c_{k,q} u_s^{k,q}(\xi, \theta).$$

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- Rewrite the forward model in transformed domain as:

$$\tilde{\zeta}_\ell = H_{\theta_\ell} c + \tilde{\varepsilon}_\ell, \quad \theta_\ell \sim p, \quad \ell \in \{1, 2, \dots, L\}$$

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Image reconstruction from truncated expansion coefficients

From the truncated expansion coefficient c , we can reconstruct the image in the spatial domain,

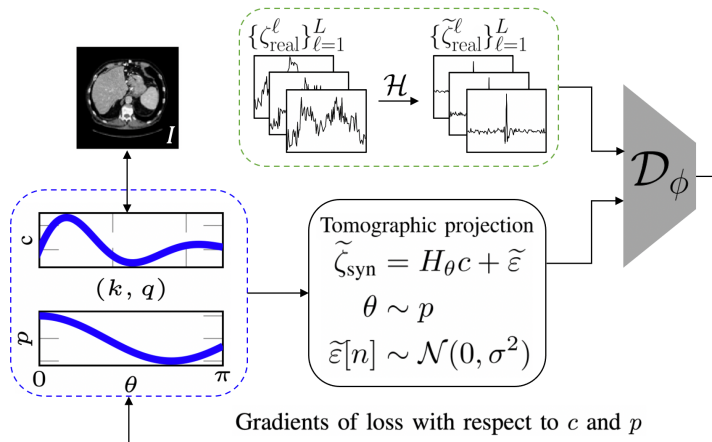
$$I(r, \varphi) = \sum_{k=-k_{\max}}^{k_{\max}} \sum_{q=1}^{p_k} c_{k,q} \mathcal{H}\left(u_s^{k,q}\right)(r, \varphi)$$

where

$$\mathcal{H}\left(u_s^{k,q}\right)(r, \varphi) = \frac{2\sqrt{2\pi}s(-1)^{(q+l)}R_{k,q}J_k(2\pi sr)}{(2\pi sr)^2 - R_{k,q}^2} \cos(k\varphi + \frac{\pi}{4}),$$

and $l = \frac{k+1}{2}$ for odd k and $l = \frac{k}{2}$ for even k .

An adversarial learning based reconstruction



Wasserstein generative adversarial learning

- Follow the Wasserstein GAN, the loss is

$$\mathcal{L}(c, p, \phi) = \sum_{b=1}^B \mathcal{D}_{\phi}(\tilde{\zeta}_{\text{real}}^b) - \mathcal{D}_{\phi}(\tilde{\zeta}_{\text{syn}}^b) + \lambda \text{GP}(\tilde{\zeta}_{\text{int}}^b)$$

- Generator loss:

$$\begin{aligned}\mathcal{L}_G(c, p) &= - \sum_{b=1}^B \mathcal{D}_{\phi}(H_{\theta_b} c + \tilde{\varepsilon}_b), \\ &= - \sum_{b=1}^B \sum_{t=1}^{N_{\theta}} \delta(\theta_t - \theta_b) \mathcal{D}_{\phi}(H_{\theta_t} c + \tilde{\varepsilon}_b), \quad \theta_b \sim p.\end{aligned}$$

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- $\mathcal{L}_G$ is non-differentiable with respect to p . How to allow backpropagation?

Approximation of the generator loss

- Discretize projection angle domain to N_θ equal bins.

¹E. Jang et al., Categorical reparameterization with Gumbel-softmax, ICLR, 2017 

Approximation of the generator loss

- Discretize projection angle domain to N_θ equal bins.
- Use Gumbel-Softmax¹ to allow backpropagation through samples from discrete distributions.

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Approximation of the generator loss

- Discretize projection angle domain to N_θ equal bins.
- Use Gumbel-Softmax¹ to allow backpropagation through samples from discrete distributions.
- Approximate $\mathcal{L}_G$ such that it is differentiable in both c and p .

¹E. Jang et al., Categorical reparameterization with Gumbel-softmax, ICLR, 2017 

Approximation of the generator loss

- The Gumbel-Max trick:

$$\delta(\theta_t - \theta_b) = \text{one hot} \left(\underset{i}{\operatorname{argmax}} [g_{b,i} + \log(p[i])] \right), g_{b,i} \sim \text{Gumbel}(0, 1)$$

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- Use softmax function as a continuous, differentiable approximation to argmax ¹:
$$r_{i,b}(p) = \frac{\exp((g_{b,i} + \log(p[i]))/\tau)}{\sum_{j=1}^{N_\theta} \exp((g_{b,j} + \log(p[j]))/\tau)}$$

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- The approximate generator loss becomes:

$$\mathcal{L}_G(c, p) \approx - \sum_{b=1}^B \sum_{i=1}^{N_\theta} r_{i,b}(p) \mathcal{D}_\phi(H_{\theta_i} c + \tilde{\varepsilon}_b).$$

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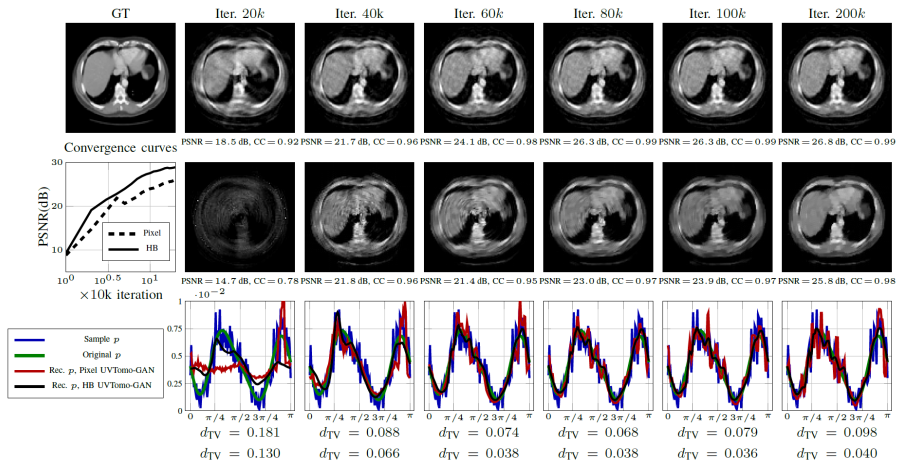
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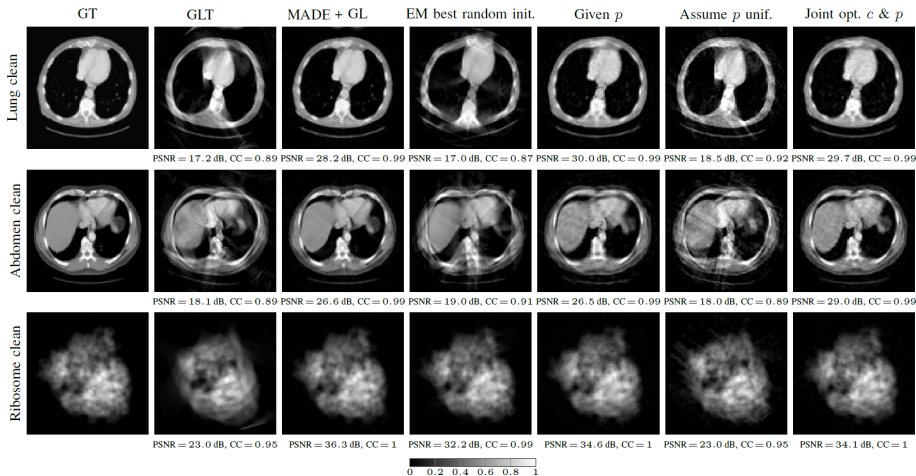
- Differentiable with respect to both c and p .

¹E. Jang et al., Categorical reparameterization with Gumbel-softmax, ICLR, 2017 

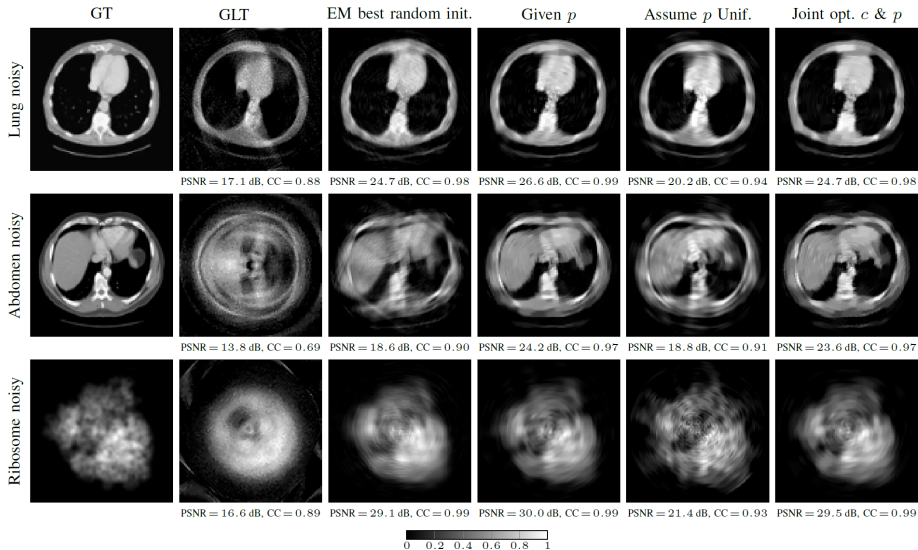
Numerical results



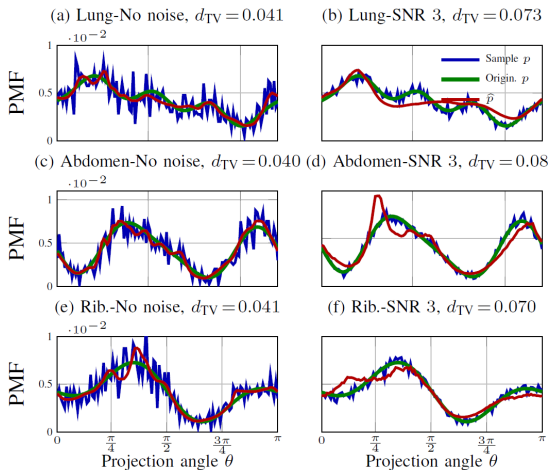
Numerical results—reconstructions from clean projections



Numerical results—at SNR= 3



Numerical results—viewing angle distribution



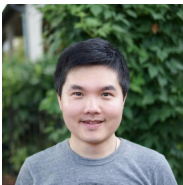
Summary and discussions

- We introduce an adversarial learning approach to jointly reconstruct image and viewing angle distribution from random 2D tomographic projections.
- To update the viewing angle distribution via backpropagation, we use Gumbel-softmax approximation of samples from categorical distribution.
- Future directions: Extend to 3D reconstruction, understand the sample complexity, adapt to different measurement uncertainty.

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Thank You!



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