Two-Dimensional Tomography from Noisy Projection Tilt Series Taken at Unknown View Angles with Non-Uniform Distribution

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Motivation & Intro: A Statistical Estimation Problem

- Unknown 2-D object $f$, and unknown non-uniform view angle distribution $p(\theta)$.
- Observation model: $y_{i,\kappa} = P_{\theta_i+\kappa\alpha}(f) + n_{i,\kappa}$, $\forall i \in [N]$, $|\kappa| \leq K$.
- Parameters of interest: $f$ and $p(\theta)$. 

Forward Model

Inverse Problem
Related Works and Problems

- **Existing methods focus on estimating view angles.**
  - S. Basu and Y. Bresler\(^1\):
    - View angle ordering via nearest neighbor;
    - Joint maximum likelihood refinement.
  - A. Singer and H. Wu\(^2\):
    - Denoising (e.g., linear Wiener filtering and graph denoising);
    - Diffusion maps for view angle ordering.
  - **Cons:** Poor performance under low SNR; Computationally inefficient with large number of projections.

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    - Diffusion maps for view angle ordering.
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- Related problems:
  - 1-D: Multi-segment reconstruction (MSR).
  - 3-D: Sub-tomogram averaging (STA) in cryo-ET and single-particle reconstruction (SPR) in cryo-EM.


Proposed Method

- Method of Moments (MoM):
  - Conjecture: first and second order moments may contain sufficient information for the recovery.
  - Difficulty: algorithm by directly inverting the first and second order moments is unavailable with unknown non-uniform view angle distribution \(p(\theta)\).
  - Solution: use nonconvex optimization methods to solve constrained weighted nonlinear least squares of first and second order moments.
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  - Solution: use nonconvex optimization methods to solve constrained weighted nonlinear least squares of first and second order moments.
  - Pros: lower computational complexity. ($N : \# \text{ of data}$)
    - MoM: $\mathcal{O}(N)$ for moments (once) and $\mathcal{O}(1)$ for each iteration.
    - MLE (e.g., EM): $\mathcal{O}(N)$ for each iteration.
Moment Features

- Fourier domain: \( \mathcal{F}(f)(\xi, \theta) \approx \sum_{k = -k_{\text{max}}}^{k_{\text{max}}} \sum_{q=1}^{q_{\text{max}}} a_{k,q} \psi_{c}^{k,q}(\xi, \theta) \).
- Fourier slice theorem: \( \hat{y}_{i,\kappa}[\xi_{j}] = \mathcal{F}(f)(\xi_{j}, \theta_{i} + \kappa \alpha) + \hat{n}_{i,\kappa}[\xi_{j}] \).
- First order moment:
  \[
  \mu[j; \kappa] = \sum_{k = -k_{\text{max}}}^{k_{\text{max}}} \sum_{q=1}^{q_{\text{max}}} a_{k,q} \psi_{c}^{k,q}(\xi_{j}, \phi_{l} + \kappa \alpha) \hat{p}[l]
  \]
  \[
  = \Psi \left( a \circ g(\hat{p}) \right)[j; \kappa].
  \]
- Second order moment:
  \[
  C[j_{1}; \kappa_{1}, j_{2}; \kappa_{2}] = \sum_{k_{1} = -k_{\text{max}}}^{k_{\text{max}}} \sum_{k_{2} = -k_{\text{max}}}^{k_{\text{max}}} \sum_{q_{1}=1}^{q_{\text{max}}} \sum_{q_{2}=1}^{q_{\text{max}}} a_{k_{1},q_{1}} a_{k_{2},q_{2}}
  \]
  \[
  \times \psi_{c}^{k_{1},q_{1}}(\xi_{j_{1}}, \kappa_{1} \alpha) \psi_{c}^{k_{2},q_{2}}(\xi_{j_{2}}, \kappa_{2} \alpha) \hat{p}[k_{2} - k_{1}]
  \]
  \[
  = (\Psi (aa^{*} \circ H(\hat{p})) \Psi^{*})[j_{1}; \kappa_{1}, j_{2}; \kappa_{2}].
  \]
Moment Features

- Unbiased empirical estimators:
  \[
  \tilde{\mu} = \frac{1}{N} \sum_{i=1}^{N} \hat{y}_i, \quad \tilde{\Sigma} = \frac{1}{N} \sum_{i=1}^{N} \hat{y}_i \hat{y}_i^* - \hat{\Sigma}.
  \]

- Constrained weighted nonlinear least squares:
  \[
  (\tilde{a}, \tilde{p}) = \arg \min_{a,p} \frac{\lambda_1}{2} \| \Psi (a \circ g(\hat{p})) - \tilde{\mu} \|^2_w + \frac{\lambda_2}{2} \| \Psi (aa^* \circ H(\hat{p})) \Psi^* - \tilde{C} \|^2_w,
  \]
  s.t. \( p \geq 0 \) and \( 1^T p = 1 \).

- Gradient based methods (e.g., gradient descent and trust region) do not work well.
An Alternating Direction Method of Multiplier (ADMM) Approach

- Reformulation and relaxation: split $a$ into $a$ and $z$, and relax the positive constraint on $p$.

$$(\tilde{a}, \tilde{p}) = \arg \min_{a,p} \frac{\lambda_1}{2} \| \Psi (a \circ g(\hat{p})) - \tilde{\mu} \|^2_w + \frac{\lambda_2}{2} \| \Psi (aa^* \circ H(\hat{p})) \psi^* - \tilde{C} \|^2_W,$$

s.t. $p \geq 0$ and $1^T p = 1$. 
An Alternating Direction Method of Multiplier (ADMM) Approach

- Reformulation and relaxation: split $a$ into $u$ and $z$, and relax the positive constraint on $p$.

$$(\tilde{a}, \tilde{z}, \tilde{p}) = \arg\min_{a, z, p} \frac{\lambda_1}{2} \| \psi(u \circ g(\hat{p})) - \tilde{\mu} \|_W^2 + \frac{\lambda_1}{2} \| \psi(z \circ g(\hat{p})) - \tilde{\mu} \|_W^2$$
$$+ \frac{\lambda_2}{2} \| \psi(az^* \circ H(\hat{p})) \psi^* - \tilde{C} \|_W^2$$

s.t. $a = z$, $p \geq 0$ and $1^\top p = 1$. 
An Alternating Direction Method of Multiplier (ADMM) Approach

- Reformulation and relaxation: split $a$ into $a$ and $z$, and relax the positive constraint on $p$.

$$(\tilde{a}, \tilde{z}, \tilde{p}) = \arg\min_{a, z, p} \frac{\lambda_1}{2} \| \Psi (a \circ g(\hat{p})) - \tilde{\mu} \|_W^2 + \frac{\lambda_1}{2} \| \Psi (z \circ g(\hat{p})) - \tilde{\mu} \|_W^2 + \frac{\lambda_2}{2} \| \Psi (az^* \circ H(\hat{p})) \Psi^* - \tilde{C} \|_W^2$$

s.t. $a = z$, $p \succeq 0$ and $1^\top p = 1$. 

$$L(a, z, p; s) = \frac{\lambda_1}{2} \| \Psi (a \circ g(\hat{p})) - \tilde{\mu} \|_W^2 + \frac{\lambda_1}{2} \| \Psi (z \circ g(\hat{p})) - \tilde{\mu} \|_W^2 + \frac{\lambda_2}{2} \| \Psi (az^* \circ H(\hat{p})) \Psi^* - \tilde{C} \|_W^2 + \rho \| a - z + s \|_2^2.$$
An Alternating Direction Method of Multiplier (ADMM) Approach

- Reformulation and relaxation: split \( a \) into \( a \) and \( z \), and relax the positive constraint on \( p \).

\[
(\tilde{a}, \tilde{z}, \tilde{p}) = \arg \min_{a, z, p} \frac{\lambda_1}{2} \| \Psi (a \circ g(\hat{p})) - \tilde{\mu} \|_W^2 + \frac{\lambda_1}{2} \| \Psi (z \circ g(\hat{p})) - \tilde{\mu} \|_W^2 + \frac{\lambda_2}{2} \| \Psi (az^* \circ H(\hat{p})) \psi^* - \tilde{C} \|_W^2
\]

s.t. \( a = z \), \( p \geq 0 \) and \( 1^T p = 1 \).

- Augmented Lagrangian:

\[
L(a, z, p; s) = \frac{\lambda_1}{2} \| \Psi (a \circ g(\hat{p})) - \tilde{\mu} \|_W^2 + \frac{\lambda_1}{2} \| \Psi (z \circ g(\hat{p})) - \tilde{\mu} \|_W^2 + \frac{\lambda_2}{2} \| \Psi (az^* \circ H(\hat{p})) \psi^* - \tilde{C} \|_W^2 + \frac{\rho}{2} \| a - z + s \|_2^2.
\]
An ADMM Approach

- Initialization: random initialization of $a^{(0)}$, $z^{(0)}$, $p^{(0)}$, and $s^{(0)} = 0$.

- Iterations: alternates between the primal updates of variables $a$, $z$, and $p$, and the dual update for $s$ until convergence.

\[
\begin{align*}
  a^{(t+1)} &= \arg \min_{a} L(a, z^{(t)}, p^{(t)}, s^{(t)}) \\
  z^{(t+1)} &= \arg \min_{z} L(a^{(t+1)}, z, p^{(t)}, s^{(t)}) \\
  p^{(t+1)} &= \arg \min_{p} L(a^{(t+1)}, z^{(t+1)}, p, s^{(t)}) \\
  s^{(t+1)} &= s^{(t)} + a^{(t+1)} - z^{(t+1)}
\end{align*}
\]

Output $a^{(t)}$, $p^{(t)}$.

Remark: each update can be realized by solving simple least squares.
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  - $a^{(t+1)} = \text{arg min}_a \mathcal{L}(a, z^{(t)}, p^{(t)}; s^{(t)})$
Initialization: random initialization of \(a^{(0)}, z^{(0)}, p^{(0)},\) and \(s^{(0)} = 0\).

Iterations: alternates between the primal updates of variables \(a, z,\) and \(p,\) and the dual update for \(s\) until convergence.

\[
\begin{align*}
\text{Iteration } t+1: \\
\quad a^{(t+1)} & = \arg\min_a \mathcal{L}(a, z^{(t)}, p^{(t)}; s^{(t)}) \\
\quad z^{(t+1)} & = \arg\min_z \mathcal{L}(a^{(t+1)}, z, p^{(t)}; s^{(t)}) \\
\quad p^{(t+1)} & = \arg\min_p \mathcal{L}(a^{(t+1)}, z^{(t+1)}, p; s^{(t)}) \\
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Output: \(a^{(t)}, p^{(t)}\).

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Output $a^{(t)}$, $p^{(t)}$.

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- Output $a^{(t)}$, $p^{(t)}$.

- Remark: each update can be realized by solving simple least squares.
Numerical Results: Clean Case

- Parameters: \( N = 10000, \alpha = 1.5 \text{ deg}, |\kappa| = 13, c = 0.3, \lambda_1 = 1, \lambda_2 = 0.5, \text{ and } \rho = 1. \)
- Exact recovery on a projection image of 70S ribosome (up to a rotation).
- Perfect match of view angle distribution (up to a rotation).

(a) Original  (b) Reconstructed  (c) \( \tilde{p}(\theta) \)
Numerical Results: Noisy Case

Figure: SNR [dB] = 6.61, -0.32, -4.38, -7.25, -9.49.

- EM algorithm for maximum marginalized log-likelihood estimation:

\[
\max_{a, p} \sum_{i=1}^{N} \ln P(\hat{y}_i|a, p) \quad \text{s.t.} \quad p \geq 0 \quad \text{and} \quad 1^T p = 1.
\]
Numerical Results: Noisy Case

Parameters: $N = 10000$, $\alpha = 3.8$ deg, $|\kappa| = 13$, $c = 0.3$, $\lambda_1 = 1$, $\lambda_2 = 5$, and $\rho = 1$.

Results over 20 independent experiments.

Performance: ADMM+EM > ADMM > EM.
Thank you!

- Our paper *Two-dimensional Tomography from Noisy Projection Tilt Series Taken at Unknown View Angles with Non-uniform Distribution* is available online at:
  https://ieeexplore.ieee.org/document/8803755

- Our codes are available online at:
  https://github.com/LingdaWang/2D_TOMO_ICIP2019