### Introduction

We try to align a set of three dimensional (3D) density functions that are randomly translated and rotated. We do not have direct access to these functions but we measure a Radon transform of these functions. Radon transform is a set of parallel line integrals of a density function taken at various projection angles. We can recover a 3D density function from the associated Radon transform using filtered back-projection method. These are called reconstructions or tomograms.

**Figure 1:** Left: Radon transform. Right: A: Transmission electron microscope sample holder rotations. B: Projection, C: Back-projection

One major complication of using a transmission electron microscope to acquire Radon transforms is that we cannot cover the entire angular range of the 3D function due to the sample holder geometry. These missing angular components are called missing wedge. Therefore, the reconstructions have distorted appearances and they are difficult to align them directly.

**Figure 2:** Left: Projection-slice theorem. Right: Effect of missing wedge in 2D

One of the most common approaches to align tomograms with missing wedge is to recover the alignment parameters that maximize the constrained correlation coefficient between the reference and the reconstructions. This approach is only valid if we have a reliable reference density function. Therefore, we need a different approach if a reference function is not available.

### Alignment problem as a matrix rank minimization problem

Given a set of Radon transforms and estimated standard deviations of noise $\sigma_i$ of each Radon transform, we have a following non-convex formulation of the alignment problem.

$$\begin{align*}
\text{minimize} & \quad \text{rank}(X) \\
\text{subject to} & \quad \|R_i(T_p(x_i)) - R_i(v_i)\|_2 \leq \sigma_i, \quad 1 \leq i \leq n
\end{align*}$$

where $X = [\text{vec}(x_1), \ldots, \text{vec}(x_n)] \in \mathbb{R}^{kn \times n}$ and $R_i(v_i) \in \mathbb{R}^{nM}$ are the observed Radon transforms, where $v_i$ is a copy of the original function that has been rotated by $(\phi_i^x, \phi_i^y, \phi_i^z)$ degrees around each axis ($x, y, z$) and translated by $(t_i^x, t_i^y, t_i^z)$ pixels along each axis. $p_i = (\phi_i^x, \phi_i^y, \phi_i^z, t_i^x, t_i^y, t_i^z)$. $R_i(T_p(x_i))$ is the rotated and translated copy of $x_i$ by the alignment parameter $p_i$.

### Sequential programming and convex relaxation

By relaxing the rank objective to the nuclear norm and linearizing the rotation and translation operator $T_p(\cdot)$, we have a following sequential convex program-

$$\begin{align*}
X(0) & \leftarrow X_0, p_i \leftarrow 0, \quad 1 \leq i \leq n \\
\text{for} \quad k = 1, \ldots, n_{\text{steps}} \quad \text{do} \\
\text{Solve the subproblem defined in Eq. 1, which returns } X \text{ and } \Delta p_i \\
X_i^{(k+1)} & \leftarrow X_i^{(k)} - \alpha \Delta p_i, \quad 1 \leq i \leq n \\
\text{end} \\
\text{and, the subproblem is} \\
\text{minimize} & \quad \|X\|_* \\
\text{subject to} & \quad \|R_i^p(x_i) - R_i(v_i)\|_2 \leq \sigma_i, \quad 1 \leq i \leq n
\end{align*}$$

where $X = [\text{vec}(x_1), \ldots, \text{vec}(x_n)] \in \mathbb{R}^{kn \times n}$ and $p_i \in \mathbb{R}^6$ are the optimization variables, $\alpha$ is a step size, and $\Delta p_i$ is the parameter updates. $R_i^p(x_i) \in \mathbb{R}^{nM \times 6}$ is a matrix whose columns are the Jacobian matrices of $T_p(x_i)$ with respect to each parameter in $p_i$. Notice that $R_i(T_p(\cdot))$ can be combined as a single linear operator $R_i^p(\cdot)$ since $p_i$ is not an optimization variable any more.

### TFOCS Approach

One way to solve the problem is to utilize the convex cone problem solver, TFOCS, developed by Becker and E. J. Candès and M. C. Grant. To utilize TFOCS, we need to re-formulate the subproblem into a conic form as below.

$$\begin{align*}
\text{minimize} & \quad \|X\|_* \\
\text{subject to} & \quad \begin{bmatrix} R_i^p(x_i) & J_p(x_i) \end{bmatrix} \begin{bmatrix} x_i \end{bmatrix} + \begin{bmatrix} b_i \end{bmatrix} \in \mathcal{K},
\end{align*}$$

where $\mathcal{K} = \{ (x, \tau) : \|x\|_2 \leq \tau \}$ and $b_i = -R_i(v_i)$. TFOCS requires three functions defined: the proximal operator of the objective function, the proximal operator of the quadratic cone, and the linear measurement operator and its adjoint. In our case, the proximal operator of the objective function is the singular value thresholding. TFOCS is a variation of the accelerated proximal gradient method discussed in the class.

### Numerical example

- 100 tomograms of $32 \times 32 \times 32$ pixels. Translated by $(t_i^x, t_i^y, t_i^z) \in [-5, 5] \times [-5, 5] \times [-5, 5]$, and rotated by $(\phi_i^x, \phi_i^y, \phi_i^z) \in [-180, 180] \times [-180, 180] \times [-180, 180]$.
- The initial translation given by mass centering, and the initial rotation is within a range of $[{-15, 15}]$ degrees from the correct value.
- Each tomogram has 25 Radon projections of 46×46 pixels. $\theta = (-60, -55, \ldots, 60)$.

### Results

1. Aligning all six parameters at once
2. Fixing the translation parameters at the mass center
3. Different initial point realization of 2.

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