Question 5, Assignment 3: CS 754, Spring 2024-25

Amitesh Shekhar
IIT Bombay
22b0014@iitb.ac.in

Anupam Rawat
IIT Bombay
22b3982@iitb.ac.in

Toshan Achintya Golla
IIT Bombay
22b2234@iitb.ac.in

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Declaration: The work submitted is our own, and we have adhered to the principles of academic honesty while completing and submitting this work. We have not referred to any unauthorized sources, and we have not used generative AI tools for the work submitted here.

1. Consider two observed particle images Q_1 and Q_2 corresponding to a 3D density map, each in different 3D orientations and 2D shifts. Let Q_1 be obtained by translating a zero-shift particle image P_1 by $(\delta_{x1}, \delta_{y1})$. Let Q_2 be obtained by translating a zero-shift particle image P_2 by $(\delta_{x2}, \delta_{y2})$. Note that Q_1, Q_2 are practically observed, whereas P_1, P_2 are not observed. Let the common line for the particle images P_1, P_2 pass through the origins of their respective coordinate systems at angles θ_1 and θ_2 with respect to their respective X axes. Derive a relationship between $\delta_{x1}, \delta_{y1}, \theta_1, \delta_{x2}, \delta_{y2}, \theta_2$ and some other observable property of the projection images. Explain how you will determine $\delta_{x1}, \delta_{y1}, \delta_{x2}, \delta_{y2}$ using this equation. Explain how you will extend this relationship to determine the shifts $\{(\delta_{xi}, \delta_{yi})\}_{i=1}^{N}$ of the N different projection images, and mention the number of knowns and unknowns. [5+2+8+3=18 points]

Soln:

We are given two observed particle images, Q_1 and Q_2, which correspond to different 2D projections of a common 3D density map. These images are obtained from their respective zero-shift versions, P_1 and P_2, but are shifted by unknown translations:

- Q_1 is obtained by shifting P_1 by $(\delta_{x1}, \delta_{y1})$.
- Q_2 is obtained by shifting P_2 by $(\delta_{x2}, \delta_{y2})$.

Note that each 2D projection of the 3D structure corresponds to a slice of the 3D Fourier transform of the object, as described by the Fourier Slice Theorem. Since these slices pass through the origin in Fourier space, any two such slices must intersect along a common 1D line. Since both P_1 and P_2 are 2D projections of the same 3D object, they share a common 1D projection line in Fourier space. Similarly, Q_1 and Q_2 share a common 1D projection line in Fourier space.

Let θ_1 and θ_2 be the angles of the common line in the coordinate systems of P_1 and P_2. Thereby we can say that the common line equation states that for all frequency magnitudes k:

$$F_1(k\cos\theta_1, k\sin\theta_1) = F_2(k\cos\theta_2, k\sin\theta_2) \tag{1}$$

where F_1 and F_2 are the Fourier transforms of the zero-shift images P_1 and P_2.

Now, we know that when an image is shifted in real space by (δ_x, δ_y), then the Fourier transform P of the given image and Fourier transform Q of the shifted image are related by a phase shift as follows:

$$F_Q(k_x, k_y) = F_P(k_x, k_y)e^{-i(k_x\delta_x + k_y\delta_y)} \tag{2}$$

Thus, the observed images Q_1 and Q_2 have Fourier transforms:

$$F_{Q_1}(k_x, k_y) = F_{P_1}(k_x, k_y)e^{-i(k_x\delta_{x1} + k_y\delta_{y1})} \tag{3}$$

$$F_{Q_2}(k_x, k_y) = F_{P_2}(k_x, k_y)e^{-i(k_x\delta_{x2} + k_y\delta_{y2})} \tag{4}$$

Using equations (1), (3) and (4), we get:

$$F_{Q_1}(k\cos\theta_1, k\sin\theta_1)e^{i(k\cos\theta_1\delta_{x1} + k\sin\theta_1\delta_{y1})} = F_{Q_2}(k\cos\theta_2, k\sin\theta_2)e^{i(k\cos\theta_2\delta_{x2} + k\sin\theta_2\delta_{y2})} \tag{5}$$

The above simplifies to:

$$k(\cos\theta_1\delta_{x1} + \sin\theta_1\delta_{y1}) = k(\cos\theta_2\delta_{x2} + \sin\theta_2\delta_{y2}) \tag{6}$$

$$\cos\theta_1\delta_{x1} + \sin\theta_1\delta_{y1} = \cos\theta_2\delta_{x2} + \sin\theta_2\delta_{y2} \tag{7}$$

Note that the equation above provides one constraint on the unknown shifts. Given multiple particle images $\{Q_i\}_{i=1}^N$, we can generalize this approach:
For any two images Q_i and Q_j:

$$\cos\theta_i\delta_{xi} + \sin\theta_i\delta_{yi} = \cos\theta_j\delta_{xj} + \sin\theta_j\delta_{yj} \tag{8}$$

For N images, there are $2N$ unknowns (δ_{xi}, δ_{yi} for each image). wherein each unique image pair gives a new equation. Forming equations for $\frac{N(N-1)}{2}$ pairs provides a system of equations that can be solved. Thus, solving this system recovers all translations (δ_{xi}, δ_{yi}).