Cryo-EM report 05/07 Definition of Extraction Matrix

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3. Liner Statistical Model

3.1 From continuous to discrete

From previous section, we have following linear image formation mode:

$$X_{ij} = CTF_{ij} \sum_{l}^{L} P_{jl}^{\phi_i} V_l + N_{ij} \tag{1}$$

where we have a clear definition of $X_{ij},\ CTF_{ij}$ and N_{ij}. Then we want to give more techniques details about extraction matrix P^{ϕ}(in our report we define, later delete this note) and 3D Fourier component V_l. This section will bring much understanding of how this linear statiscal model is derived.

Again, we start from Projection Slice Theorem, it gives us straightforward connection between points in 2D fourier space and correspoinding points in 3D space.

$$X_i(\omega_1,\ \omega_2,\ 0) = CTF(\omega_1, \omega_2,\ 0) V_C(R_i^{-1} \underset{\sim}{\omega}) + N_{ij} \tag{2}$$

where $X_i = F\varphi_R$ is the 2D Fourier Transformation of the ith experiment image. $V_C = F\varphi$, is the 3D Fourier transformation of 3D structure $\varphi(\underset{\sim}{x})$. Therefore V_C remains continuous and we denote its subscript C. $R_i \in SO(3)$ is the rotation matrix for the ith image. Still $\underset{\sim}{\omega} = (\omega_1, \omega_2, 0)$ is as we previously defined. Again, this equation means a 2D projectd Fourier image is equal to a central slice of 3D Fourier Transformation image. But in reality it is filtered by CTF and will be plus noise N_{ij}.

(1) Because the $i$the experiment image X_i^r is a digital image in real experiment, we can only take sampled discrete grid points from X_i^r. (2) On the other hand, we can only do Discrete Fourier Transformation in computer. Due to above two reasrons, 2D Fourier Transformed image X_i should be discrete and represents in matrix form. $(\omega_1,\ \omega_2,\ 0)$ then would also be in discrete case. At the same time, we notice $CTF(\omega_1, \omega_2, 0)$ has the same argument $(\omega_1, \omega_2, 0)$ as X_i. Thus, we write equation (2) in another way:

$$X_{ij} = CTF_{ij} V_C(R_i^{-1} \underset{\sim}{\omega}) + N_{ij}$$

where we use j to define a specific $(\omega_1,\ \omega_2,\ 0)$, which means jth component in Fig.3 of manuscript ABA. Specifically, given j we will directly know the value of $\underset{\sim}{\omega}$ because j fixed the coordinates of $\underset{\sim}{\omega}$ accordding to 2D Discrete Fourier Transformation gridding method.

In addion to that, discreteness in computing will lead to another problem shown in Fig.1 and Fig.2. For each projected X_i, each grid point of it may not match the grid point in 3D Fourier space.

Secondly, there are a large amount of projections and we cannot garantee them to be uniform distributed in 3D Fourier space. In other words, if we put all these slices back to their true locations in 3D Fourier space, there must be some area has denser points and some area has sparse points. In conlusion, after we put each slice to its right location in 3D Fourier space, we would have a large amount of points $\{V_l\}$ which are non-uniform distributed and not orderd. We would use XXXX interpolation method to get ordered grid points in 3D Fourier space. To stress it again, we want to estimate the intensity values of each V_l.

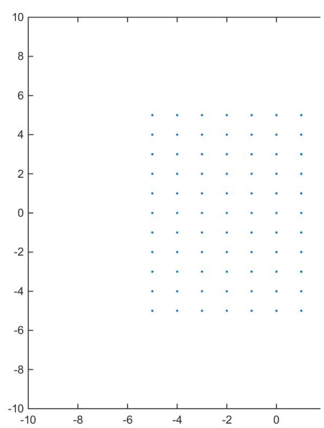

Fig.2 2D Fourier grid space

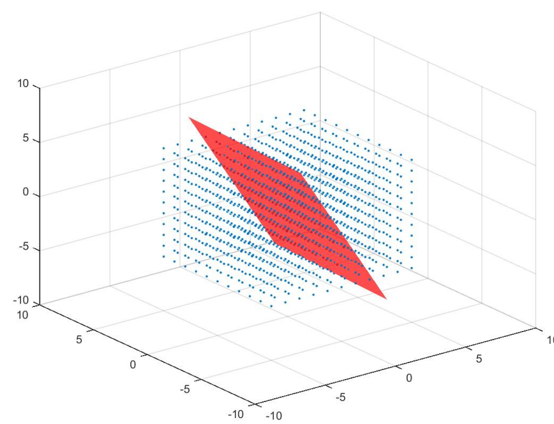

Fig.2 3D Fourier grid space with a central slice

3.2 Extraction of slice

Next we move from equation (2) to equation (1) and compare $V_C(R_i^{-1}\underset{\sim}{\omega})$ and $\sum_l^L P_{jl}^{\phi_i} V_l$,which are the same. What $\sum_l^L P_{jl}^{\phi_i} V_l$ is doing is as follows: (1) First we assume there are $L = I \times J$ 3D Fourier components $\{V_l\}$. Each compoents corresponds to one components of one 2D image X_i. We order set $\{V_l\}$ accordding to image i and in-image index j. Since $\{V_l\}$ is a $1 \times L$ vector, we denote the elements from the ith section, which is $((i-1) \times J + 1)$th element to $(i \times J)$th element, as correspoding elements from the ith image X_i, for $i = 1, 2, \cdots, I$. Furthermore, if given rotation matrix parameters ϕ_i for $i = 1, 2, \cdots, I$, we would know specific coordinate of each element is $\{V_l\}$. For example, in ith section, the coordinate of $((i-1) \times J + j)$th component is $R_i^{-1}(\omega_{1,j}, \omega_{2,j}, 0)$, where $\omega_{1,j}$ and $\omega_{2,j}$ can be determined if we know j .

Here we denote coordinate set for ith section as

$$\begin{aligned} C_i &= \{C_{i,1}, C_{i,2}, \cdots,\ C_{i,J}\} \\ &= \{R_i^{-1}(\omega_{1,1}, \omega_{2,1}, 0),\ ,\cdots,\ R_i^{-1}(\omega_{1,J}, \omega_{2,J}, 0)\} \end{aligned} \tag{3}$$

for $i = 1, 2, \cdots, I$.

(2) Then $\underset{\sim}{P_j^{\phi}} = (P_{j1}^{\phi_i},\ P_{j2}^{\phi_i},\ ,\cdots,\ P_{jL}^{\phi_i})$ would be a very sparse matrix. We define it as

$$P_{jk}^{\phi_i} = \begin{cases} 0 & if\ k \neq ((i-1) \times J + j) \\ 1 & if\ k = ((i-1) \times J + j) \end{cases},\ for\ k = 1,\ \cdots,\ L \tag{4}$$

Intuitively,

$$\underset{\sim}{P_j^{\phi_i}} = (0,\ 0,\ \cdots,\ 1,\ 0, \cdots,\ 0)_{1 \times L} \tag{5}$$

with the $((i-1) \times J + j)$th element being 1 and all other elements being 0.

So there would be I extraction matrix $(P^{\phi_i})_{J \times L}$ for $i = 1, \cdots,\ I$. Following the definition of formula (3),

$$P^{\phi_i} = \begin{bmatrix} 0 & \cdots & 1 & 0 & \cdots & & & & 0 \\ 0 & & & 1 & 0 & \cdots & & & 0 \\ 0 & & & & 1 & \cdots & & & 0 \\ \vdots & & & & & \ddots & & & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & & 1 & \cdots & 0 \end{bmatrix}_{J \times L}$$

All in all, the operation of $\sum_l^L P_{jl}^{\phi_i} V_l$ is selecting a component V_l , with $l = (i-1) \times J + j$ in our definition, while suppress all other components V_k for $k \neq l$ to be 0. Accordding to Projection Slice Theorem, this V_l with coordinate $(R_i^{-1}(\omega_{1,j}, \omega_{2,j}, 0))$ should be equal to X_{ij} theoretically, if not consider CTF and noise.