Bayesian approach to tomographic reconstruction

The reconstruction problem is formulated as finding the model with parameter set Θ that has the highest probability of being the correct one in the light of both the observed data X and the prior information Y. According to Bayes' law, this so-called posterior distribution factorizes into two components:

$$P(\Theta|X,Y) \propto P(X|\Theta,Y)P(\Theta|Y) \tag{1}$$

where the *likelihood* $P(X|\Theta,Y)$ quantifies the probability of observing the data given the model, and the *prior* $P(\Theta|Y)$ expresses how likely that model is given the prior information.

Over here, we use a linear image formation model in the Fourier space:

$$X_{ij} = CTF_{ij} \sum_{l=1}^{L} P^{\phi}_{jl} V_l + N_{ij} \tag{2}$$

where,

- X_{ij} is the j^{th} component, with $j = 1, 2, .., J$ of the one-dimensional (1D) Fourier transform of the i^{th} experimental projection, with $i = 1, 2.., N$.
- CTF_{ij} is the j^{th} component of the contrast transfer function for the i^{th} image.
- V_l is the l^{th} component, with $l = 1, 2, .., L$ of the 2D Fourier transform V of the underlying structure in the data set.
- $\mathbf{P}^{\phi}$ is a $J \times L$ matrix of elements P^{ϕ}_{jl}. The operation $\sum_{l=1}^{L} P^{\phi}_{jl} V_l$ for all j extracts a slice out of the 3D Fourier transform of the underlying structure. Similarly, the operation $\sum_{j=1}^{J} P^{\phi^T_{lj}} X_{ij}$ for all l places the 1D Fourier transform of an experimental projection back into the 2D transform.

The projection operator $\mathbf{P}^{\phi}$ or equivalently its back-projection operation (which is a transpose of $\mathbf{P}^{\phi}$ - $\mathbf{P}^{\phi^{\mathbf{T}}}$) has several interesting properties,

- $\sum_{l=1}^{L} P^{\phi}_{jl} = 1$ or $\sum_{j=1}^{J} P^{\phi}_{jl} = 1$
- $\sum_{j=1}^{J} P^{\phi^T_{lj}} = 1$ or $\sum_{l=1}^{L} P^{\phi^T_{lj}} = 1$
- $\mathbf{P}^{\phi}$ has just one non-zero element in each row and column which is equal to 1.
-
$$\sum_{j=1}^{J} P^{\phi}_{jl^*} \sum_{l=1}^{L} P^{\phi}_{jl} V_l = \sum_{j=1}^{J} P^{\phi}_{jl^*} V_{l^*} \tag{3}$$

  This is am important formula which is going to be used later. To prove it, lets consider a j'. We know $P^{\phi}_{j'l}$ is one for only one value of l, say l' and for rest all its zero. Therefore for j' the expression is $P^{\phi}_{j'l^*} V_{l'}$ which just evaluates to 0 as P_{jl^*} is only 1 for $P_{j^*l^*}$ and for rest all its zero. Thus we get the result as mentioned above

Or we can equivalently write,

$$V_l = \sum_{j=1}^{J} \frac{P^{\phi^T_{lj}}}{CTF_{ij}} (X_{ij} - N_{ij}) \tag{4}$$

We assume that all the noise components N_{ij} are independent and Gaussian distributed. The variance σ^2_{ij} of these noise components is unknown and must be estimated from the data. The assumption of independence in the noise allows the probability of observing an image given its orientation and the model to be calculated as a multiplication of Gaussians over all its Fourier components:

$$P(X_i|\phi,\Theta,Y) = \prod_{j=1}^{J} \frac{1}{2\pi\sigma^2_{ij}} exp\left(\frac{|X_{ij} - CTF_{ij} \sum_{l=1}^{L} P^{\phi}_{jl} V_l|^2}{-2\sigma^2_{ij}} \right) \tag{5}$$

The corresponding marginal likelihood of observing the entire data set X is then given by:

$$P(X|\Theta, Y) = \prod_{i=1}^{N} \int_{\phi} P(X_i|\phi, \Theta, Y)P(\phi|\Theta, Y)d\phi \tag{6}$$

where $P(\phi|\Theta, Y)$ expresses prior information about the distribution of orientations.

Calculation of the prior relies on the assumption of smoothness in the reconstruction. Smoothness is encoded in the assumption that all Fourier components V_l are independent and Gaussian distribution with zero mean and unknown variance τ_l^2, so that:

$$P(\Theta|Y) = \prod_{l=1}^{L} \frac{1}{2\pi\tau_l^2} exp\left(\frac{|V_l^2|}{-2\tau_l^2}\right) \tag{7}$$

We use expectation maximization to find the optimal values of V_l^2, τ_l^2, and σ_{ij}^2. For the expectation maximization algorithm we treat the orientation (Φ) of all the projections as hidden variables. In the *E-step* of the algorithm we basically have to compute the conditional expectation $E_{\mathbf{\Phi}|\mathbf{X},\Theta_n} lnP(\mathbf{X}, \phi|\Theta)$. Next, in the *M-step*, we maximize this expression along with the prior with respect to Θ.

$$E_{\mathbf{\Phi}|\mathbf{X},\Theta_n} lnP(\mathbf{X}, \phi|\Theta) = \int_{\phi} P(\phi|\mathbf{X}, \Theta_n) lnP(\mathbf{X}, \phi|\Theta)d\phi \tag{8}$$

First lets have a look at $P(\phi|\mathbf{X}, \Theta_n)$ and try to express it in quantities we know.

$$\begin{aligned} P(\phi|\mathbf{X}, \Theta_n) &= \frac{P(\phi, \mathbf{X}, \Theta_n)}{P(\mathbf{X}, \Theta)} \\ &= \frac{P(\mathbf{X}|\phi, \Theta_n)P(\phi|\Theta_n)}{P(\mathbf{X}|\Theta_n)} \end{aligned} \tag{9}$$

Lets say that,

$$\Gamma_{i\phi}^n = \frac{P(X_i|\phi, \Theta_n)P(\phi|\Theta_n)}{P(X_i|\Theta_n)} \tag{10}$$

Therefore,

$$P(\phi|\mathbf{X}, \Theta_n) = \prod_{i=1}^{N} \Gamma_{i\phi}^n = K_\phi^n \tag{11}$$

Now lets have a look at $P(\mathbf{X}, \phi|\Theta)$,

$$\begin{aligned} P(\mathbf{X}, \phi|\Theta) &= P(\mathbf{X}|\phi, \Theta)P(\phi|\Theta) \\ &= \prod_{i=1}^{N} P(X_i|\phi, \Theta)P(\phi|\Theta) \end{aligned} \tag{12}$$

Now we can rewrite Eqn 8 as,

$$E_{\mathbf{\Phi}|\mathbf{X},\Theta_n} lnP(\mathbf{X}, \phi|\Theta) = \int_{\phi} \prod_{i=1}^{N} \Gamma_{i\phi}^n \sum_{i=1}^{N} lnP(X_i|\phi, \Theta) + lnP(\phi|\Theta)d\phi \tag{13}$$

Substituting the value of $P(X_i|\phi, \Theta)$ we get,

$$E_{\mathbf{\Phi}|\mathbf{X},\Theta_n} lnP(\mathbf{X}, \phi|\Theta) = \int_{\phi} K_\phi^n \sum_{i=1}^{N} ln \prod_{j=1}^{J} \frac{1}{2\pi\sigma_{ij}^2} exp\left(\frac{|X_{ij} - CTF_{ij} \sum_{l=1}^{L} P_{jl}^{\phi} V_l|^2}{-2\sigma_{ij}^2}\right) d\phi \tag{14}$$

which on simplification equals,

$$
\begin{aligned}
&= \int_\phi K_\phi^n \sum_{i=1}^N \sum_{j=1}^J ln \frac{1}{2\pi\sigma_{ij}^2} exp\left(\frac{|X_{ij} - CTF_{ij} \sum_{l=1}^L P_{jl}^\phi V_l|^2}{-2\sigma_{ij}^2} \right) d\phi \\
&= \int_\phi K_\phi^n \sum_{i=1}^N \sum_{j=1}^J -ln(2\pi\sigma_{ij}^2) + \frac{|X_{ij} - CTF_{ij} \sum_{l=1}^L P_{jl}^\phi V_l|^2}{-2\sigma_{ij}^2} d\phi
\end{aligned}
\tag{15}
$$

In the maximization step, we try to maximize the following expression with respect to V_l^2, τ_l^2, and σ_{ij}^2. Note that $lnP(\Theta|Y)$ represents our prior and is being utilized in the maximization step.

$$
\begin{aligned}
&= \arg \max_{V_{l^*}, \tau_{l^*}, \sigma_{ij}} E_{\mathbf{\Phi}|\mathbf{X},\Theta_n} lnP(\mathbf{X}, \phi|\Theta) + lnP(\Theta|Y) \\
&= \arg \max_{V_{l^*}, \tau_{l^*}, \sigma_{ij}} \int_\phi K_\phi^n \sum_{i=1}^N \sum_{j=1}^J -ln(2\pi\sigma_{ij}^2) + \frac{|X_{ij} - CTF_{ij} \sum_{l=1}^L P_{jl}^\phi V_l|^2}{-2\sigma_{ij}^2} d\phi + \sum_{l=1}^L ln \frac{1}{2\pi\tau_l^2} exp\left(\frac{|V_l|^2}{-2\tau_l^2} \right) \\
&= \arg \max_{V_{l^*}, \tau_{l^*}, \sigma_{ij}} \int_\phi K_\phi^n \sum_{i=1}^N \sum_{j=1}^J -ln(2\pi\sigma_{ij}^2) + \frac{|X_{ij} - CTF_{ij} \sum_{l=1}^L P_{jl}^\phi V_l|^2}{-2\sigma_{ij}^2} d\phi + \sum_{l=1}^L -ln 2\pi\tau_l^2 + \frac{|V_l|^2}{-2\tau_l^2}
\end{aligned}
\tag{16}
$$

First we will differentiate this with respect to V_{l^*} to find the optimal value for the next iteration. Differentiating and equating it to zero we get,

$$
\begin{aligned}
\int_\phi K_\phi^n \sum_{i=1}^N \sum_{j=1}^J \frac{(X_{ij} - CTF_{ij} \sum_{l=1}^L P_{jl}^\phi V_l) CTF_{ij} P_{jl^*}^\phi}{\sigma_{ij}^2} d\phi - \frac{V_{l^*}}{\tau_{l^*}^2} = 0 \\
\int_\phi K_\phi^n \sum_{i=1}^N \sum_{j=1}^J \frac{P_{jl^*}^\phi CTF_{ij} X_{ij}}{\sigma_{ij}^2} - \frac{P_{jl^*}^\phi CTF_{ij}^2 \sum_{l=1}^L P_{jl}^\phi V_l}{\sigma_{ij}^2} d\phi - \frac{V_{l^*}}{\tau_{l^*}^2} = 0
\end{aligned}
\tag{17}
$$

$$
\begin{aligned}
\int_\phi K_\phi^n \sum_{i=1}^N \sum_{j=1}^J \frac{P_{jl^*}^\phi CTF_{ij} X_{ij}}{\sigma_{ij}^2} d\phi = \int_\phi K_\phi^n \sum_{i=1}^N \sum_{j=1}^J \frac{P_{jl^*}^\phi CTF_{ij}^2 \sum_{l=1}^L P_{jl}^\phi V_l}{\sigma_{ij}^2} d\phi + \frac{V_{l^*}}{\tau_{l^*}^2} \\
\sum_{i=1}^N \int_\phi K_\phi^n \sum_{j=1}^J \frac{P_{jl^*}^\phi CTF_{ij} X_{ij}}{\sigma_{ij}^2} d\phi = \sum_{i=1}^N \int_\phi K_\phi^n \sum_{j=1}^J \frac{P_{jl^*}^\phi CTF_{ij}^2 \sum_{l=1}^L P_{jl}^\phi V_l}{\sigma_{ij}^2} d\phi + \frac{V_{l^*}}{\tau_{l^*}^2}
\end{aligned}
\tag{18}
$$

Using 3, we can simplify this expression to the following -

$$
\begin{aligned}
\sum_{i=1}^N \int_\phi K_\phi^n \sum_{j=1}^J \frac{P_{jl^*}^\phi CTF_{ij} X_{ij}}{\sigma_{ij}^2} d\phi = \sum_{i=1}^N \int_\phi K_\phi^n \sum_{j=1}^J \frac{P_{jl^*}^\phi CTF_{ij}^2 V_{l^*}}{\sigma_{ij}^2} d\phi + \frac{V_{l^*}}{\tau_{l^*}^2} \\
\sum_{i=1}^N \int_\phi K_\phi^n \sum_{j=1}^J P^{\phi_{jl^*}^T} \frac{CTF_{ij} X_{ij}}{\sigma_{ij}^2} d\phi = V_{l^*} \sum_{i=1}^N \int_\phi K_\phi^n \sum_{j=1}^J P^{\phi_{jl^*}^T} \frac{CTF_{ij}^2}{\sigma_{ij}^2} d\phi + \frac{V_{l^*}}{\tau_{l^*}^2}
\end{aligned}
\tag{19}
$$

Thus we can find the optimal value of V_{l^*} as

$$
V_{l^*} = \frac{\sum_{i=1}^N \int_\phi K_\phi^n \sum_{j=1}^J P^{\phi_{jl^*}^T} \frac{CTF_{ij} X_{ij}}{\sigma_{ij}^2} d\phi}{\sum_{i=1}^N \int_\phi K_\phi^n \sum_{j=1}^J P^{\phi_{jl^*}^T} \frac{CTF_{ij}^2}{\sigma_{ij}^2} d\phi + \frac{1}{\tau_{l^*}^2}}
\tag{20}
$$

Now that we have found the optimal value of V_l, we next move ahead with differentiating Eqn 16 with respect to τ_{l^*}. Differentiating and setting it to zero we get,

$$
-\frac{2}{\tau_{l^*}} + \frac{|V_{l^*}|^2}{\tau_{l^*}^3} = 0
\tag{21}
$$

$$
\tau_{l^*}^2 = \frac{1}{2} |V_{l^*}|^2
\tag{22}
$$

Thus we have obtained the optimal value of τ^2_{l*}. Now we have to just differentiate Eqn 16 with respect to the last parameter to σ_{ij} to complete the expectation maximization iteration. Differentiating the expression with respect to σ_{ij} we get,

$$\begin{aligned} \int_\phi K^n_\phi \sum_{i=1}^{N} \sum_{j=1}^{J} -\frac{2}{\sigma^*_{ij}} + \frac{|X_{ij} - CTF_{ij} \sum_{l=1}^{L} P^\phi_{jl} V_l|^2}{\sigma^{3*}_{ij}} d\phi = 0 \\ \sum_{i=1}^{N} \sum_{j=1}^{J} \int_\phi K^n_\phi \left(-\frac{2}{\sigma^*_{ij}} + \frac{|X_{ij} - CTF_{ij} \sum_{l=1}^{L} P^\phi_{jl} V_l|^2}{\sigma^{3*}_{ij}} \right) d\phi = 0 \end{aligned} \tag{23}$$

Since the noise is independently distributed for each projection and for each component, it makes sense to say that,

$$\begin{aligned} \int_\phi K^n_\phi \left(-\frac{2}{\sigma^*_{ij}} + \frac{|X_{ij} - CTF_{ij} \sum_{l=1}^{L} P^\phi_{jl} V_l|^2}{\sigma^{3*}_{ij}} \right) d\phi = 0 \\ -\frac{2}{\sigma^*_{ij}} + \frac{1}{\sigma^{3*}_{ij}} \int_\phi K^n_\phi |X_{ij} - CTF_{ij} \sum_{l=1}^{L} P^\phi_{jl} V_l|^2 d\phi = 0 \end{aligned} \tag{24}$$

which gives us the value of σ^*_{ij} as,

$$\sigma^*_{ij} = \frac{1}{2} \int_\phi K^n_\phi |X_{ij} - CTF_{ij} \sum_{l=1}^{L} P^\phi_{jl} V_l|^2 d\phi \tag{25}$$