

Tensor tomography gradients, uniaxial modelDefinitions and precalculations

$$\vec{r} = (x, y, z)^T \quad \text{lab coordinates}$$

$$\vec{r}_s = (x_s, y_s, z_s)^T \quad \text{sample coordinates}$$

$$R_n^{\exp(\alpha, \beta)} = \begin{bmatrix} \cos \beta & \sin \alpha \cos \beta & -\cos \alpha \sin \beta \\ 0 & \cos \alpha & \sin \alpha \\ \sin \beta & -\cos \beta \sin \alpha & \cos \alpha \cos \beta \end{bmatrix}$$

$$\left(R_n^{\exp(\alpha, \beta)}\right)^{-1} = \begin{bmatrix} \cos(-\beta) & \sin(-\alpha) \cos(-\beta) & -\cos(-\alpha) \sin(-\beta) \\ 0 & \cos(-\alpha) & \sin(-\alpha) \\ \sin(-\beta) & -\cos(-\beta) \sin(-\alpha) & \cos(\alpha) \cos(-\beta) \end{bmatrix}$$

$$= \begin{bmatrix} \cos \beta & -\sin \alpha \cos \beta & \cos \alpha \sin \beta \\ 0 & \cos \alpha & -\sin \alpha \\ -\sin \beta & \cos \beta \sin \alpha & \cos \alpha \cos \beta \end{bmatrix}$$

$$\vec{r}_s = R_n^{\exp} \vec{r} = \begin{bmatrix} x \cos \beta + y \sin \alpha \cos \beta - z \cos \alpha \sin \beta \\ y \cos \alpha + z \sin \alpha \\ x \sin \beta - y \cos \beta \sin \alpha + z \cos \alpha \cos \beta \end{bmatrix}$$

(2)

$$\vec{r} = (R_n \exp)^{-1} \vec{r}_s = \begin{bmatrix} x_s \cos \beta - y_s \sin \alpha \cos \beta + z_s \cos \alpha \sin \beta \\ y_s \cos \alpha - z_s \sin \alpha \\ x_s \sin \beta + y_s \cos \beta \sin \alpha + z_s \cos \alpha \cos \beta \end{bmatrix}$$

$$\vec{q} = (q_x, q_y, q_z)^T = \begin{bmatrix} q \sin \Theta \cos \Phi \\ q \sin \Theta \sin \Phi \\ q \cos \Theta \end{bmatrix}$$

Reciprocal space lab  
coordinates

$$\vec{q}_s = (q_{s,x}, q_{s,y}, q_{s,z})^T = \begin{bmatrix} q_s \sin \Theta_s \cos \Phi_s \\ q_s \sin \Theta_s \sin \Phi_s \\ q_s \cos \Theta_s \end{bmatrix}$$

Reciprocal space  
sample coordinate  
system

$$\vec{q}_{vox} = (q_{vox,x}, q_{vox,y}, q_{vox,z})^T = \begin{bmatrix} q_{vox} \sin \Theta \cos \Phi \\ q_{vox} \sin \Theta \sin \Phi \\ q_{vox} \cos \Theta \end{bmatrix}$$

Voxel reciprocal  
space coord  
system.

$$R^{str}(\vec{r}_s) = \begin{bmatrix} \cos \Theta_{op}(\vec{r}_s) \cos \varphi_{op}(\vec{r}_s) & \cos \Theta_{op}(\vec{r}_s) \sin \varphi_{op}(\vec{r}_s) & -\sin \Theta_{op}(\vec{r}_s) \\ -\sin \varphi_{op}(\vec{r}_s) & \cos \varphi_{op}(\vec{r}_s) & 0 \\ \sin \Theta_{op}(\vec{r}_s) \cos \varphi_{op}(\vec{r}_s) & \sin \Theta_{op}(\vec{r}_s) \sin \varphi_{op}(\vec{r}_s) & \cos \Theta_{op}(\vec{r}_s) \end{bmatrix}$$

$$\text{and } \vec{q}_{vox} = R^{str}(\vec{r}_s) \vec{q}_s = R^{str}(\vec{r}_s) R_n \exp(\alpha, \beta) \vec{q}$$



(3)

$$\vec{q}_{\text{vox}}(\vec{r}_s) = R^{\text{str}}(\vec{r}_s) R_n^{\text{exp}}(\alpha, \beta) \vec{q}$$

$$\begin{bmatrix} \sin \Theta \cos \Phi \\ \sin \Theta \sin \Phi \\ \cos \Theta \end{bmatrix} = \begin{bmatrix} \cos \Theta_{\text{op}} \cos \varphi_{\text{op}} & \cos \Theta_{\text{op}} \sin \varphi_{\text{op}} & -\sin \varphi_{\text{op}} \\ -\sin \varphi_{\text{op}} & \cos \varphi_{\text{op}} & 0 \\ \sin \Theta_{\text{op}} \cos \varphi_{\text{op}} & \sin \Theta_{\text{op}} \sin \varphi_{\text{op}} & \cos \Theta_{\text{op}} \end{bmatrix} \begin{bmatrix} \cos \beta & \sin \alpha \cos \beta & -\cos \alpha \sin \beta \\ 0 & \cos \alpha & \sin \alpha \\ \sin \beta & -\cos \beta \sin \alpha & \cos \alpha \cos \beta \end{bmatrix} \times \begin{bmatrix} \sin \Theta \cos \varphi \\ \sin \Theta \sin \varphi \\ \cos \Theta \end{bmatrix}$$

$$\begin{aligned} \cos \Theta &= [\sin \Theta_{\text{op}} \cos \varphi_{\text{op}} \cos \beta + \cos \Theta_{\text{op}} \sin \beta] \sin \Theta \cos \varphi \\ &+ [\sin \Theta_{\text{op}} \cos \varphi_{\text{op}} \sin \alpha \cos \beta + \sin \Theta_{\text{op}} \sin \varphi_{\text{op}} \cos \alpha - \cos \Theta_{\text{op}} \cos \beta \sin \alpha] \\ &\times \sin \Theta \sin \varphi \\ &+ [-\sin \Theta_{\text{op}} \cos \varphi_{\text{op}} \cos \alpha \sin \beta + \sin \Theta_{\text{op}} \sin \varphi_{\text{op}} \sin \alpha + \cos \Theta_{\text{op}} \cos \alpha \cos \beta] \\ &\times \cos \Theta \end{aligned}$$

$$\cos \Theta \Big|_{\Theta=\frac{\pi}{2}} = [\sin \Theta_{\text{op}} \cos \varphi_{\text{op}} \cos \beta + \cos \Theta_{\text{op}} \sin \beta] \cos \varphi + [\sin \Theta_{\text{op}} \cos \varphi_{\text{op}} \sin \alpha \cos \beta + \sin \Theta_{\text{op}} \sin \varphi_{\text{op}} \cos \alpha - \cos \Theta_{\text{op}} \cos \beta \sin \alpha] \sin \varphi$$

$$\begin{aligned} \sin^2 \Theta(\vec{r}_s) \Big|_{\Theta=\frac{\pi}{2}} &= 1 - \cos^2 \Theta(\vec{r}_s) \Big|_{\Theta=\frac{\pi}{2}} \\ &= 1 - \left\{ [\sin \Theta_{\text{op}}(\vec{r}_s) \cos \varphi_{\text{op}}(\vec{r}_s) \cos \beta + \cos \Theta_{\text{op}}(\vec{r}_s) \sin \beta] \cos \varphi \right. \\ &\quad \left. + [\sin \Theta_{\text{op}}(\vec{r}_s) \cos \varphi_{\text{op}}(\vec{r}_s) \sin \alpha \cos \beta + \sin \Theta_{\text{op}}(\vec{r}_s) \sin \varphi_{\text{op}}(\vec{r}_s) \cos \alpha - \cos \Theta_{\text{op}}(\vec{r}_s) \cos \beta \sin \alpha] \sin \varphi \right\}^2 \end{aligned}$$

(4)

$$\varepsilon_q = 2 \sum_{n, x, y, q} \left\{ [\hat{I}_n(x, y, q, \varphi)]^{\frac{1}{2}} - [I_n(x, y, q, \varphi)]^{\frac{1}{2}} \right\}^2$$

$$\hat{I}_n(x, y, q, \varphi) = \sum_z (A(\vec{r}_s, q))^2 e^{-B(\vec{r}_s, q) \sin^2 \Theta(\vec{r}_s, q) |_{\Theta=\frac{\pi}{2}}}$$

Calculation of gradients.

Leaving out  $q$ -dependency and mask  $w_n(x, y, q)$  and  $M(\vec{r}_s)$   
Also leaving out absorption correction  $T_n(x, y)$

$$\frac{\partial \varepsilon}{\partial A(\vec{r}_s')} = \frac{\partial}{\partial A(\vec{r}_s')} 2 \sum_{n, x, y, q} \left\{ [\hat{I}_n(x, y, q)]^{\frac{1}{2}} - [I_n(x, y, q)]^{\frac{1}{2}} \right\}^2$$

$$= 2 \sum_{n, x, y, q} 2 \left\{ [I_n(x, y, q)]^{\frac{1}{2}} - [\hat{I}_n(x, y, q)]^{\frac{1}{2}} \right\} \frac{\partial}{\partial A(\vec{r}_s')} [\hat{I}_n(x, y, q)]^{\frac{1}{2}}$$

$$= 2 \sum_{n, x, y, q} \left\{ \frac{[\hat{I}_n(x, y, q)]^{\frac{1}{2}} - [I_n(x, y, q)]^{\frac{1}{2}}}{[\hat{I}_n(x, y, q)]^{\frac{1}{2}}} \right\} \frac{\partial \hat{I}_n(x, y, q)}{\partial A(\vec{r}_s')}$$

$BP_n(x, y, q)$  (backprojection)

$$= 2 \sum_{n, x, y, q} BP_n(x, y, q) \frac{\partial}{\partial A(\vec{r}_s')} \sum_z (A(\vec{r}_s))^2 e^{-B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s) |_{\Theta=\frac{\pi}{2}}}$$

$$= 2 \sum_{n, q} \sum_{x, y, z} BP_n(x, y, q) e^{-B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s) |_{\Theta=\frac{\pi}{2}}} \frac{\partial}{\partial A(\vec{r}_s')} (A(\vec{r}_s))^2$$

$$= 2 \sum_{n, q} \sum_{x, y, z} BP_n(x, y, q) e^{-B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s) |_{\Theta=\frac{\pi}{2}}} 2 A(\vec{r}_s) \delta_{\vec{r}_s, \vec{r}_s'}$$



(5)

$$= 2 \sum_{n, \ell} \sum_{x_s, y_s, z_s} B P_n (x_s \cos \beta - y_s \sin \alpha \cos \beta + z_s \cos \alpha \cos \beta, y_s \cos \alpha - z_s \sin \alpha, \ell)$$

$$x_s e^{-B(x_s, y_s, z_s) \sin^2 \Theta(x_s, y_s, z_s)} \Big|_{\Theta = \frac{\pi}{2}} 2 A(x_s, y_s, z_s) \delta_{\vec{r}_s, \vec{r}_s}$$

$$= 4 \sum_{n, \ell} B P_n (x'_s \cos \beta - y'_s \sin \alpha \cos \beta + z'_s \cos \alpha \cos \beta, y'_s \cos \alpha - z'_s \sin \alpha, \ell)$$

$$x'_s e^{-B(x'_s, y'_s, z'_s) \sin^2 \Theta(x'_s, y'_s, z'_s)} \Big|_{\Theta = \frac{\pi}{2}} A(x'_s, y'_s, z'_s)$$

$$= 4 \sum_{n, \ell} B P(x'_s, y'_s, \ell) A(x'_s, y'_s, z'_s) e^{-B(x'_s, y'_s, z'_s) \sin^2 \Theta(x'_s, y'_s, z'_s)} \Big|_{\Theta = \frac{\pi}{2}}$$

$$\frac{\partial \varepsilon}{\partial A(\vec{r}_s)} = 4 \sum_{n, \ell} \left\{ \frac{[\hat{I}_n(x, y, \ell)]^{\frac{1}{2}} - [I_n(x, y, \ell)]^{\frac{1}{2}}}{[\hat{I}_n(x, y, \ell)]^{\frac{1}{2}}} \right\} A(\vec{r}_s) e^{-B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s)} \Big|_{\Theta = \frac{\pi}{2}}$$


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(6)

$$\frac{\partial \varepsilon}{\partial B(\vec{r}_s')} = \frac{\partial}{\partial B(\vec{r}_s')} 2 \sum_{n, x, y, q} \left\{ \frac{[\hat{I}_n(x, y, q)]^{\frac{1}{2}} - [I_n(x, y, q)]^{\frac{1}{2}}}{[\hat{I}_n(x, y, q)]^{\frac{1}{2}}} \right\}^2$$

= ... The first steps are similar as for  $\frac{\partial \varepsilon}{\partial A(\vec{r}_s)}$  ...

$$= 2 \sum_{n, x, y, q} B P_n(x, y, q) \sum_z (A(\vec{r}_s))^2 \frac{\partial}{\partial B(\vec{r}_s')} e^{-B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s)} \Big|_{\Theta=\frac{\pi}{2}}$$

$$= 2 \sum_{n, q} \sum_{x, y, z} B P_n(x, y, q) (A(\vec{r}_s))^2 e^{-B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s)} \Big|_{\Theta=\frac{\pi}{2}}$$

$$\times (-\sin^2 \Theta(\vec{r}_s)) \frac{\partial B(\vec{r}_s)}{\partial B(\vec{r}_s')}$$

$$= 2 \sum_{n, q} \sum_{x_s, y_s, z_s} B P_n(x_s \cos \beta - y_s \sin \alpha \cos \beta + z_s \cos \alpha \cos \beta, y_s \cos \alpha - z_s \sin \alpha, q)$$

$$\times (A(x_s, y_s, z_s))^2 e^{-B(x_s, y_s, z_s) \sin^2 \Theta(x_s, y_s, z_s)} \Big|_{\Theta=\frac{\pi}{2}}$$

$$\times (-\sin^2 \Theta(x_s, y_s, z_s)) \Big|_{\Theta=\frac{\pi}{2}} \delta_{\vec{r}_s, \vec{r}_s'}$$

$$= -2 \sum_{n, q} B P_n(x', y') (A(\vec{r}_s'))^2 \sin^2 \Theta(\vec{r}_s') \Big|_{\Theta=\frac{\pi}{2}}$$

$$\times e^{-B(\vec{r}_s') \sin^2 \Theta(\vec{r}_s') \Big|_{\Theta=\frac{\pi}{2}}}$$

↙ ? lost



(7)

$$\frac{\partial \mathcal{E}}{\partial B(\vec{r}_s)} = -2 \sum_{n, q} \left\{ \frac{[\hat{I}_n(x, y, q)]^{\frac{1}{2}} - [I_n(x, y, q)]^{\frac{1}{2}}}{[\hat{I}_n(x, y, q)]^{\frac{1}{2}}} \right\}$$

$$A^2 \times \sin^2 \Theta(\vec{r}_s) \Big|_{\Theta=\frac{\pi}{2}} \leftarrow -B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s) \Big|_{\Theta=\frac{\pi}{2}}$$


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$$\frac{\partial \mathcal{E}}{\partial \Theta_q(\vec{r}_s')} = \frac{\partial}{\partial \Theta_q(\vec{r}_s')} 2 \sum_{n, x, y, q} \left\{ \frac{[\hat{I}_n(x, y, q)]^{\frac{1}{2}} - [I_n(x, y, q)]^{\frac{1}{2}}}{[\hat{I}_n(x, y, q)]^{\frac{1}{2}}} \right\}^2$$

$$= \dots \text{again similar to } \frac{\partial \mathcal{E}}{\partial A(\vec{r}_s)}$$

$$= 2 \sum_{n, x, y, q} B P_n(x, y, q) \sum_z (A(\vec{r}_s))^2 \frac{\partial}{\partial \Theta_q(\vec{r}_s')} \leftarrow -B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s) \Big|_{\Theta=\frac{\pi}{2}}$$

$$= \sum_{n, q} \sum_{x, y, z} B P_n(x, y, q) (A(\vec{r}_s))^2 \leftarrow -B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s) \Big|_{\Theta=\frac{\pi}{2}}$$

$$\times (-2 B(\vec{r}_s) \sin \Theta(\vec{r}_s)) \cos \Theta(\vec{r}_s) \Big|_{\Theta=\frac{\pi}{2}} \frac{\partial \Theta(\vec{r}_s)}{\partial \Theta_q(\vec{r}_s')}$$

$$= -4 \sum_{n, q} \sum_{x, y, z} B P_n(x, y, q) (A(\vec{r}_s))^2 B(\vec{r}_s) \sin \Theta(\vec{r}_s) \Big|_{\Theta=\frac{\pi}{2}} \cos \Theta(\vec{r}_s) \Big|_{\Theta=\frac{\pi}{2}} \\ \times \leftarrow -B(\vec{r}_s) \sin \Theta(\vec{r}_s) \Big|_{\Theta=\frac{\pi}{2}} \frac{\partial \Theta(\vec{r}_s)}{\partial \Theta_q(\vec{r}_s')} \delta_{\vec{r}_s, \vec{r}_s'}$$

$$= -4 \sum_{n, q} \sum_{x, y, z} B P_n(x, y, z, \dots, q) (A(\vec{r}_s))^2 B(\vec{r}_s) \sin \Theta(\vec{r}_s) \Big|_{\theta=\frac{\pi}{2}}$$

$$\times \cos \Theta(\vec{r}_s) \Big|_{\theta=\frac{\pi}{2}} e^{-B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s) \Big|_{\theta=\frac{\pi}{2}}} \frac{\partial \Theta(\vec{r}_s) \Big|_{\theta=\frac{\pi}{2}}}{\partial \Theta_{op}(\vec{r}_s)} \int_{\vec{r}_s, \vec{r}_s'}$$

$$= -4 \sum_{n, q} \left\{ \frac{[\hat{I}_n(x, y, q)]^{\frac{1}{2}} - [I_n(x, y, q)]^{\frac{1}{2}}}{[\hat{I}_n(x, y, q)]^{\frac{1}{2}}} \right\}$$

$$\times (A(\vec{r}_s'))^2 B(\vec{r}_s') \sin^2 \Theta(\vec{r}_s') \Big|_{\theta=\frac{\pi}{2}} \cos \Theta(\vec{r}_s') \Big|_{\theta=\frac{\pi}{2}}$$

$$\times e^{-B(\vec{r}_s') \sin^2 \Theta(\vec{r}_s') \Big|_{\theta=\frac{\pi}{2}}} \frac{\partial \Theta(\vec{r}_s') \Big|_{\theta=\frac{\pi}{2}}}{\partial \Theta_{op}(\vec{r}_s')}$$

$$\frac{\partial \mathcal{E}}{\partial \Theta_{op}(\vec{r}_s)} = -4 \sum_{n, q} \left\{ \frac{[\hat{I}_n(x, y, q)]^{\frac{1}{2}} - [I_n(x, y, q)]^{\frac{1}{2}}}{[\hat{I}_n(x, y, q)]^{\frac{1}{2}}} \right\} (A(\vec{r}_s))^2 B(\vec{r}_s) \sin \Theta(\vec{r}_s) \Big|_{\theta=\frac{\pi}{2}}$$

$$\times \cos \Theta(\vec{r}_s) \Big|_{\theta=\frac{\pi}{2}} e^{-B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s) \Big|_{\theta=\frac{\pi}{2}}} \frac{\partial \Theta(\vec{r}_s) \Big|_{\theta=\frac{\pi}{2}}}{\partial \Theta_{op}(\vec{r}_s)}$$

Are these expressions correct? For  $\frac{\partial \mathcal{E}}{\partial Q_{op}}$  I assume the derivation

is identical as for  $\frac{\partial \mathcal{E}}{\partial \Theta_{op}}$ , but with  $\frac{\partial \Theta \Big|_{\theta=\frac{\pi}{2}}}{\partial Q_{op}}$  in the end.

I also assume that I can use the existing expressions

for  $\frac{\partial \Theta \Big|_{\theta=\frac{\pi}{2}}}{\partial \Theta_{op}}$  and  $\frac{\partial \Theta \Big|_{\theta=\frac{\pi}{2}}}{\partial Q_{op}}$  given by Eq. 13a and 15a

in Liebi et al, Acta Cryst 2018.