F. K. Mürer

Tensor tomography gradients, uniaxial model

Definitions and precalculations

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

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

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

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

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

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

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

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

Reciprocal space lab coordinates

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

Reciprocal space sample coordinate system

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

Voxel reciprocal space coord system.

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

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

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

$$\begin{bmatrix} \sin\Theta\cos\Phi \\ \sin\Theta\sin\Phi \\ \cos\Theta \end{bmatrix} = \begin{bmatrix} \cos\theta_{op}\cos\varphi_{op} & \cos\theta_{op}\sin\varphi_{op} & -\sin\varphi_{op} \\ -\sin\varphi_{op} & \cos\varphi_{op} & 0 \\ \sin\theta_{op}\cos\varphi_{op} & \sin\theta_{op}\sin\varphi_{op} & \cos\theta_{op} \end{bmatrix} \begin{bmatrix} \cos\beta & \sin\alpha\cos\beta & -\cos\alpha\sin\beta \\ 0 & \cos\alpha & \sin\alpha \\ \sin\beta & -\cos\beta\sin\alpha & \cos\alpha\cos\beta \end{bmatrix}$$

$$\times \begin{bmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{bmatrix}$$

$$\cos\Theta = [\sin\theta_{op}\cos\varphi_{op}\cos\beta + \cos\theta_{op}\sin\beta]\sin\theta\cos\varphi$$

$$+[\sin\theta_{op}\cos\varphi_{op}\sin\alpha\cos\beta + \sin\theta_{op}\sin\varphi_{op}\cos\alpha - \cos\theta_{op}\cos\beta\sin\alpha]$$

$$\times\sin\theta\sin\varphi$$

$$+[-\sin\theta_{op}\cos\varphi_{op}\cos\alpha\sin\beta + \sin\theta_{op}\sin\varphi_{op}\sin\alpha + \cos\theta_{op}\cos\alpha\cos\beta]$$

$$\times\cos\theta$$

$$\cos\Theta\Big|_{\theta=\frac{\pi}{2}} = [\sin\theta_{op}\cos\varphi_{op}\cos\beta + \cos\theta_{op}\sin\beta]\cos\varphi$$

$$+[\sin\theta_{op}\cos\varphi_{op}\sin\alpha\cos\beta + \sin\theta_{op}\sin\varphi_{op}\cos\alpha$$

$$-\cos\theta_{op}\cos\beta\sin\alpha]\sin\varphi$$

$$\sin^2\Theta(\vec{r}_s)\Big|_{\theta=\frac{\pi}{2}} = 1 - \cos^2\Theta(\vec{r}_s)\Big|_{\theta=\frac{\pi}{2}}$$

$$= 1 - \{[\sin\theta_{op}(\vec{r}_s)\cos\varphi_{op}(\vec{r}_s)\cos\beta + \cos\theta_{op}(\vec{r}_s)\sin\beta]\cos\varphi$$

$$+[\sin\theta_{op}(\vec{r}_s)\cos\varphi_{op}(\vec{r}_s)\sin\alpha\cos\beta \pm \sin\theta_{op}(\vec{r}_s)\sin\varphi_{op}(\vec{r}_s)\cos\alpha$$

$$-\cos\theta_{op}(\vec{r}_s)\cos\beta\sin\alpha]\sin\varphi\}^2$$

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

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

<u>Calculation of gradients.</u>

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

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

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

$$= 2\sum_{n,x,y,\varphi} \underbrace{\left\{ \frac{\left[\hat{I}_n(x,y,\varphi)\right]^{\frac{1}{2}} - \left[I_n(x,y,\varphi)\right]^{\frac{1}{2}}}{\left[\hat{I}_n(x,y,\varphi)\right]^{\frac{1}{2}}} \right\}}_{BP_n(x,y,\varphi)\ \text{(backprojection)}} \frac{\partial \hat{I}_n(x,y,\varphi)}{\partial A(\vec{r}_s^{\,\prime})}$$

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

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

$$= 2\sum_{n,\varphi}\sum_{x,y,z} BP_n(x,y,\varphi)\, e^{-B(\vec{r}_s)\sin^2\Theta(\vec{r}_s)\big|_{\Theta=\frac{\pi}{2}}}\, 2A(\vec{r}_s)\, \delta^3_{\vec{r}_s, \vec{r}_s^{\,\prime}}$$

$$= 2 \sum_{n,\varphi} \sum_{x_s, y_s, z_s s} BP_n\left(x_s \cos\beta - y_s \sin\alpha \cos\beta + z_s \cos\alpha \cos\beta \,,\, y_s \cos\alpha - z_s \sin\alpha, \varphi\right)$$

$$\times\, e^{-B(x_s, y_s, z_s)\sin^2 \Theta(x_s, y_s, z_s)}\Big|_{\Theta = \frac{\pi}{2}} \; 2A(x_s, y_s, z_s)\, \delta^3_{\vec{r}_s, \vec{r}_s'}$$

$$= 4 \sum_{n,\varphi} BP_n\left(x_s' \cos\beta - y_s' \sin\alpha \cos\beta + z_s' \cos\alpha \cos\beta, y_s' \cos\alpha - z_s' \sin\alpha, \varphi\right)$$

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

$$= 4 \sum_{n,\varphi} BP(x', y', \varphi)\, A(x_s', y_s', z_s')\, e^{-B(x_s', y_s', z_s')\sin^2 \Theta(x_s', y_s', z_s')}\Big|_{\Theta = \frac{\pi}{2}}$$

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

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

$= \ldots$ The first steps are similar as for $\dfrac{\partial \mathcal{E}}{\partial A(\vec{r}_s)}$ $\ldots$

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

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

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

$$= 2\sum_{n,\varphi}\sum_{x_s,y_s,z_s} BP_n(x_s\cos\beta - y_s\sin\alpha\cos\beta + z_s\cos\alpha\cos\beta,\; y_s\cos\alpha - z_s\sin\alpha,\; \varphi)$$

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

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

$$= -2\sum_{n,\varphi} BP_n(x',y')\left(A(\vec{r}_s')\right)^2 \sin^2\Theta(\vec{r}_s')\Big|_{\Theta=\frac{\pi}{2}}$$

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

? Lost

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

$$A^2 \times \sin^2 \Theta(\vec{r}_s)\big|_{\theta=\frac{\pi}{2}}\, e^{-B(\vec{r}_s)\sin^2\Theta(\vec{r}_s)\big|_{\theta=\frac{\pi}{2}}}$$

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

$= \ldots$ again similar to $\frac{\partial \varepsilon}{\partial A(\vec{r}_s)}$

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

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

$$\times\,(-2B(\vec{r}_s)\sin\Theta(\vec{r}_s))\cos\Theta(\vec{r}_s)\big|_{\Theta=\frac{\pi}{2}}\;\frac{\partial\Theta(\vec{r}_s)}{\partial\Theta_{cp}(\vec{r}_s')}$$

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

$$\times\; e^{-B(\vec{r}_s)\sin\Theta(\vec{r}_s)\big|_{\theta=\frac{\pi}{2}}}\;\frac{\partial\Theta(\vec{r}_s)}{\partial\Theta_{cp}(\vec{r}_s)}\;\delta_{\vec{r}_s,\vec{r}_s'}$$

$$= -4 \sum_{n,\varphi} \sum_{x_s,y_s,z_s} BP_n(x_s \cos\beta \ldots, \ldots, \varphi)\, |A(\vec{r}_s)|^2 B(\vec{r}_s) \sin \Theta(\vec{r}_s)\Big|_{\theta=\frac{\pi}{2}}$$

$$\times \cos \Theta(\vec{r}_s)\Big|_{\theta=\frac{\pi}{2}}\, e^{-B(\vec{r}_s) \sin^2 \Theta(\vec{r}_s)|_{\theta=\frac{\pi}{2}}}\, \frac{\partial \Theta(\vec{r}_s)|_{\theta=\frac{\pi}{2}}}{\partial \Theta_{op}(\vec{r}_s')}\, \delta^3_{\vec{r}_s, \vec{r}_s'}$$

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

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

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

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

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

Are these expressions correct? For $\frac{\partial \varepsilon}{\partial \varphi_{op}}$ I assume the derivation is identical as for $\frac{\partial \varepsilon}{\partial \Theta_{op}}$, but with $\frac{\partial \Theta|_{\theta=\frac{\pi}{2}}}{\partial \varphi_{op}}$ in the end.

I also assume that I can use the existing expressions for $\frac{\partial \Theta}{\partial \Theta_{op}}\Big|_{\theta=\frac{\pi}{2}}$ and $\frac{\partial \Theta}{\partial \varphi_{op}}\Big|_{\theta=\frac{\pi}{2}}$ given by Eq. 13a and 15a in Liebi et al, Acta Cryst 2018.