Prediction parameter gradients

Calculating the detector coordinates of a Bragg spot

Let $\vec{R}$ be the vector from the center of the Ewald sphere to the reciprocal lattice point. The radius of the Ewald sphere is k_{pred}, which is $1/\lambda$ for monochromatic radiation. For wide-bandwidth radiation, take the wavelength which excites the reflection.

$$\vec{R} = \begin{pmatrix} x_l \\ y_l \\ z_l + k_{\mathrm{pred}} \end{pmatrix},$$

where

$$\begin{pmatrix} x_l \\ y_l \\ z_l \end{pmatrix} = \begin{pmatrix} a_x^* & a_y^* & a_z^* \\ b_x^* & b_y^* & b_z^* \\ c_x^* & c_y^* & c_z^* \end{pmatrix} \begin{pmatrix} h \\ k \\ l \end{pmatrix}.$$

The direction of $\vec{R}$ in reciprocal space is the same as the direction of the diffracted ray. The diffracted ray intersects the detector panel at pixel coordinates (X, Y). Let the corner of the panel be $\vec{C}$, and the fast and slow scan basis vectors $\vec{f}$ and $\vec{s}$ respectively. We can write:

$$\mu\vec{R} = \vec{C} + X\vec{f} + Y\vec{s},$$

or equivalently in matrix form:

$$\mu\vec{R} = \begin{pmatrix} c_x & f_x & s_x \\ c_y & f_y & s_y \\ c_z & f_z & s_z \end{pmatrix} \begin{pmatrix} 1 \\ X \\ Y \end{pmatrix} = \hat{M} \begin{pmatrix} 1 \\ X \\ Y \end{pmatrix}.$$

Dividing both sides by μ gives:

$$\vec{R} = \hat{M} \begin{pmatrix} 1/\mu \\ X/\mu \\ Y/\mu \end{pmatrix} = \hat{M}\vec{P},$$

which can be solved for X and Y. Since there are usually a large number of reflections, it may be better to calculate and store the inverse of $\hat{M}$ and calculate $\vec{P} = \hat{M}^{-1}\vec{R}$ (as of version 0.11.1, CrystFEL does not do this).

Gradients of spot position

We seek ${}^{d}/_{d\bullet}(X)$ and ${}^{d}/_{d\bullet}(Y)$, where $\bullet$ represents any parameter (e.g. c_y, f_x, a_z^*). Start by calculating ${}^{d}/_{d\bullet}(\vec{P})$ and therefore ${}^{d}/_{d\bullet}({}^{X}/_{\mu})$ and ${}^{d}/_{d\bullet}({}^{Y}/_{\mu})$, as well as ${}^{d}/_{d\bullet}({}^{1}/_{\mu})$. The required gradients can then be calculated using the product rule:

$$\frac{d(X/\mu)}{d\bullet} = \frac{1}{\mu}\frac{dX}{d\bullet} + X\frac{d(1/\mu)}{d\bullet},$$

rearranging to get

$$\frac{dX}{d\bullet} = \mu\left[\frac{d(X/\mu)}{d\bullet} - X\frac{d(1/\mu)}{d\bullet}\right],$$

and similarly for Y. To calculate ${}^{d}/_{d\bullet}(\vec{P})$, apply the product rule as follows:

$$\frac{d\vec{P}}{d\bullet} = \frac{d}{d\bullet}(\hat{M}^{-1}\vec{R}) = \hat{M}^{-1}\frac{d\vec{R}}{d\bullet} + \frac{d\hat{M}^{-1}}{d\bullet}\vec{R}.$$

This separates the gradients into terms which depend on the detector geometry ($\frac{d\hat{M}^{-1}}{d\bullet}$) and terms which depend on the diffraction physics ($\frac{d\vec{R}}{d\bullet}$).

Detector geometry terms

Convert the derivative of the inverse matrix into the derivative of the original matrix using:

$$\frac{d}{d\bullet}\hat{M}^{-1} = -M^{-1}\frac{d\hat{M}}{d\bullet}M^{-1}.$$

Physics terms

The gradients of $\vec{R}$ are calculated in vector form by routine ray_vector_gradient() inside CrystFEL. The gradient with respect to the reciprocal axis length $|a^*|$ is

$$\frac{d\vec{R}}{d\,|\vec{a}^*|} = \frac{h\vec{a}^*}{|\vec{a}^*|},$$

and similarly for $|b^*|$ and $|c^*|$. The vector gradients of $\vec{R}$ with respect to rotations around x, y and z are respectively

$$\begin{pmatrix} 0 \\ -z_l \\ y_l \end{pmatrix}, \begin{pmatrix} z_l \\ 0 \\ -x_l \end{pmatrix}, \begin{pmatrix} -y_l \\ x_l \\ 0 \end{pmatrix}.$$

The gradients of $\vec{R}$ with respect to reciprocal inter-axial angles α^*, β^* and γ^* are calculated starting with the following conventions:

- Increasing α^* rotates the b^* axis around $c^* \wedge b^*$.
- Increasing β^* rotates the c^* axis around $a^* \wedge c^*$.
- Increasing γ^* rotates the a^* axis around $b^* \wedge a^*$.

All rotations follow the right hand grip rule convention. For small rotations, the general rotation matrix is

$$\begin{pmatrix} 1 & -\theta u_z & \theta u_y \\ \theta u_z & 1 & -\theta u_x \\ -\theta u_y & \theta u_x & 1 \end{pmatrix},$$

where (u_x, u_y, u_z) is the rotation axis and θ is the small rotation angle. The gradient of this matrix with respect to θ is simply

$$\begin{pmatrix} 0 & -u_z & u_y \\ u_z & 0 & -u_x \\ -u_y & u_x & 0 \end{pmatrix},$$

which leads to the following gradients (in each case with the axis defined as listed above):

$$\begin{aligned} \frac{d\vec{R}}{d\alpha^*} &= -k\left(u_z b_y^* + u_y b_z^*\right), \\ \frac{d\vec{R}}{d\beta^*} &= -l\left(u_z c_y^* + u_y c_z^*\right), \\ \frac{d\vec{R}}{d\gamma^*} &= -h\left(u_z a_y^* + u_y a_z^*\right). \end{aligned}$$

Gradients of excitation error

The excitation error is defined as $1/\lambda - \left|\vec{R}\right|$. The gradient of excitation error is therefore

$$\begin{aligned} -\frac{d}{d\bullet}\left|\vec{R}\right| &= -\frac{d}{d\bullet}\left[\left|\vec{R}\right|^2\right]^{1/2} = -\frac{d}{d\bullet}\left[x_l^2 + y_l^2 + z_l^2 + \frac{2z_l}{\lambda} + \frac{1}{\lambda^2}\right]^{1/2} \\ &= -\frac{1}{2\left|\vec{R}\right|}\left[\frac{d(x_l^2)}{d\bullet} + \frac{d(y_l^2)}{d\bullet} + \frac{d(z_l^2)}{d\bullet} + \frac{2}{\lambda}\frac{dz_l}{d\bullet}\right] \\ &= -\frac{1}{2\left|\vec{R}\right|}\left[2x_l\frac{dx_l}{d\bullet} + 2y_l\frac{dy_l}{d\bullet} + 2z_l\frac{dz_l}{d\bullet} + \frac{2}{\lambda}\frac{dz_l}{d\bullet}\right] \\ &= -\frac{1}{\left|\vec{R}\right|}\begin{pmatrix} dx_l/d\bullet \\ dy_l/d\bullet \\ dz_l/d\bullet \end{pmatrix}\cdot\vec{R}. \end{aligned}$$

We assume that λ is a constant, so:

$$\begin{pmatrix} dx_l/d\bullet \\ dy_l/d\bullet \\ dz_l/d\bullet \end{pmatrix} = \frac{d\vec{R}}{d\bullet},$$

which allows the formulae from the previous section to be re-used.