

Dear Jerome and Jonathan,

We were struggling with rietveld refining some textured diffraction patterns, that made us look at the polarization and solid angle corrections of the integration. Here we noticed that the integrated intensity is corrected using the integrated correction. According to the *next generation* formulation:

$$I_{\text{bin}} = \frac{\sum_{\text{pix} \in \text{bin}} c_{\text{bin}}^{\text{pix}} I_{\text{pix}}}{\sum_{\text{pix} \in \text{bin}} c_{\text{pix}}^{\text{pix}} \Omega_{\text{pix}} P_{\text{pix}}} \quad (1)$$

We do not understand this, as textured signals should see a different polarization correction based on the direction that the peak is oriented in.

We do understand your concern for error propagation though, but looking into it a bit further, we see you have two error propagation methods, one for the *next generation* integration shown in eq. (1):

$$\sigma_{\text{bin}} = \frac{\sqrt{\sum_{\text{pix} \in \text{bin}} (c_{\text{bin}}^{\text{pix}})^2 \sigma_{\text{pix}}^2}}{\sum_{\text{pix} \in \text{bin}} c_{\text{bin}}^{\text{pix}} \Omega_{\text{pix}} P_{\text{pix}}} \quad (2)$$

In contrast to this, the *legacy* methods were as follows:

$$I_{\text{bin}} = \frac{\sum_{\text{pix} \in \text{bin}} c_{\text{bin}}^{\text{pix}} \frac{I_{\text{pix}}}{\Omega_{\text{pix}} P_{\text{pix}}}}{\sum_{\text{pix} \in \text{bin}} c_{\text{bin}}^{\text{pix}}} \quad (3)$$

$$\sigma_{\text{bin}} = \frac{\sqrt{\sum_{\text{pix} \in \text{bin}} c_{\text{bin}}^{\text{pix}} \sigma_{\text{pix}}^2}}{\sum_{\text{pix} \in \text{bin}} c_{\text{bin}}^{\text{pix}}} \quad (4)$$

Note that while the corrections are applied in the error of the *next generation* integration method, eq. (2), neither the solid angle correction nor the polarization corrections are applied in the *legacy* method (eq. (4)). Looking through the code on the readthedocs page: “Variance of SAXS data” on the pyFAI site, we noticed that  $\sigma_{\text{pix}}$  includes the intensity, but *not* the corrections.

Thus we suggest that the old *legacy* of integrating was in fact correct, but that the error should instead have been propagated as follows:

$$\sigma_{\text{bin}} = \frac{\sqrt{\sum_{\text{pix} \in \text{bin}} (c_{\text{bin}}^{\text{pix}})^2 \frac{\sigma_{\text{bin}}^2}{(\Omega_{\text{bin}} P_{\text{bin}})^2}}}{\sum_{\text{pix} \in \text{bin}} c_{\text{bin}}^{\text{pix}}} \quad (5)$$

Or a combination of eqs. (3) and (5). In our testing, this allows for correct corrections of the data, while also not shifting the  $\chi^2$  distribution.

Best regards,

The MAX IV Diffraction & Scattering group