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Bulk-solvent and overall scaling revisited: faster calculations, improved results. Corrigendum.

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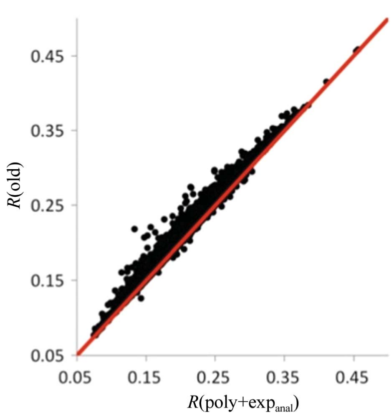
Equations in Sections 2.3 and 2.4 of the article by Afonine *et al.* [*Acta Cryst.* (2013). **D69**, 625–634] are corrected.



In the article by Afonine *et al.* (2013) some improper notations and errors in several equations in Sections 2.3 and 2.4 have been corrected. We note that the *Computational Crystallography Toolbox* (Grosse-Kunstleve *et al.*, 2002) has been using the correct version of these equations since 2013. Updated versions of Section 2.3 and equations (42), (43) and (45) are given below.

2.3. Bulk-solvent parameters and overall isotropic scaling

Assuming the resolution-dependent scale factors $k_{\rm mask}(\mathbf{s})$ and $k_{\rm isotropic}(\mathbf{s})$ to be constants $k_{\rm mask}$ and $k_{\rm isotropic}$ in each thin resolution shell, the determination of their values is reduced to minimizing the residual

$$\sum_{\mathbf{s}}\{|\mathbf{F}_{\rm calc}(\mathbf{s})+k_{\rm mask}\mathbf{F}_{\rm mask}(\mathbf{s})|^2 - [k_{\rm overall}\,k_{\rm anisotropic}(\mathbf{s})k_{\rm isotropic}]^{-2}F^2_{\rm obs}(\mathbf{s})\}^2, \quad (22)$$

where the sum is calculated over all reflections $\mathbf{s}$ in the given resolution shell, and $k_{\rm overall}$ and $k_{\rm anisotropic}(\mathbf{s})$ are calculated previously and fixed. This minimization problem is generally highly over-determined because the number of reflections per shell is usually much larger than two.

Introducing $w_{\mathbf{s}} = |\mathbf{F}_{\rm mask}(\mathbf{s})|^2$, $v_{\mathbf{s}} = \frac{1}{2}[\mathbf{F}_{\rm calc}(\mathbf{s})\mathbf{F}^*_{\rm mask}(\mathbf{s}) + \mathbf{F}^*_{\rm calc}(\mathbf{s})\mathbf{F}_{\rm mask}(\mathbf{s})]$, $u_{\mathbf{s}} = |\mathbf{F}_{\rm calc}(\mathbf{s})|^2$, $I_{\mathbf{s}} = [k_{\rm overall}\,k_{\rm anisotropic}(\mathbf{s})]^{-2}F^2_{\rm obs}(\mathbf{s})$ and $K = k^{-2}_{\rm isotropic}$ and substituting them into (22) leads to the minimization of

$$\mathrm{LS}(K, k_{\rm mask}) = \sum_{\mathbf{s}}[(k^2_{\rm mask}w_{\mathbf{s}} + 2k_{\rm mask}v_{\mathbf{s}} + u_{\mathbf{s}}) - KI_{\mathbf{s}}]^2 \quad (23)$$

with respect to K and $k_{\rm mask}$. This leads to a system of two equations:

$$\left\{\begin{aligned} \frac{\partial}{\partial K}\mathrm{LS}(K, k_{\rm mask}) &= -2\sum_{\mathbf{s}}[(k^2_{\rm mask}w_{\mathbf{s}} + 2k_{\rm mask}v_{\mathbf{s}} + u_{\mathbf{s}}) - KI_{\mathbf{s}}]I_{\mathbf{s}} \\ &= 0, \\ \frac{\partial}{\partial k_{\rm mask}}\mathrm{LS}(K, k_{\rm mask}) &= 4\sum_{\mathbf{s}}[(k^2_{\rm mask}w_{\mathbf{s}} + 2k_{\rm mask}v_{\mathbf{s}} + u_{\mathbf{s}}) - KI_{\mathbf{s}}] \\ &\quad\times(k_{\rm mask}w_{\mathbf{s}} + v_{\mathbf{s}}) \\ &= 0. \end{aligned}\right. \quad (24)$$

Developing these equations with respect to $k_{\rm mask}$,

$$\begin{cases} k_{\rm mask}^2 \sum\limits_{\bf s} w_{\bf s} I_{\bf s} + 2k_{\rm mask} \sum\limits_{\bf s} v_{\bf s} I_{\bf s} + \sum\limits_{\bf s} u_{\bf s} I_{\bf s} - K \sum\limits_{\bf s} I_{\bf s}^2 = 0, \\ k_{\rm mask}^3 \sum\limits_{\bf s} w_{\bf s}^2 + 3k_{\rm mask}^2 \sum\limits_{\bf s} w_{\bf s} v_{\bf s} + k_{\rm mask} \sum\limits_{\bf s} (2v_{\bf s}^2 + u_{\bf s} w_{\bf s} - K I_{\bf s} w_{\bf s}) \\ \qquad + \sum\limits_{\bf s} u_{\bf s} v_{\bf s} - K \sum\limits_{\bf s} I_{\bf s} v_{\bf s} = 0, \end{cases} \tag{25}$$

and introducing new notations for the coefficients, we obtain

$$\begin{cases} k_{\rm mask}^2 C_2 + k_{\rm mask} B_2 + A_2 - K Y_2 = 0, \\ k_{\rm mask}^3 D_3 + k_{\rm mask}^2 C_3 + k_{\rm mask}(B_3 - K C_2) + A_3 - K Y_3 = 0. \end{cases} \tag{26}$$

Multiplying the second equation by Y_2 and substituting KY_2 from the first equation into the new second equation, we obtain a cubic equation with fixed coefficients

$$k_{\rm mask}^3 (D_3 Y_2 - C_2^2) + k_{\rm mask}^2 (C_3 Y_2 - C_2 B_2 - C_2 Y_3) + k_{\rm mask}(B_3 Y_2 - C_2 A_2 - Y_3 B_2) + (A_3 Y_2 - Y_3 A_2) = 0. \tag{27}$$

The senior coefficient in equation (27) satisfies the Cauchy–Schwarz inequality:

$$D_3 Y_2 - C_2^2 = \sum_{\bf s} w_{\bf s}^2 \sum_{\bf s} I_{\bf s}^2 - \sum_{\bf s} w_{\bf s} I_{\bf s} \sum_{\bf s} w_{\bf s} I_{\bf s} > 0. \tag{28}$$

Therefore, equation (27) can be rewritten as

$$k_{\rm mask}^3 + a k_{\rm mask}^2 + b k_{\rm mask} + c = 0 \tag{29}$$

and solved using a standard procedure.

The corresponding values of K are obtained by substituting the roots of equation (29) into the first equation in equation (26),

$$K = (k_{\rm mask}^2 C_2 + k_{\rm mask} B_2 + A_2)/Y_2. \tag{30}$$

If no positive root exists, $k_{\rm mask}$ is assigned a zero value, which implies the absence of a bulk-solvent contribution. If several roots with $k_{\rm mask} \geq 0$ exist then the one that gives the smallest value of LS(K, $k_{\rm mask}$) is selected.

If desired, one can fit the right-hand side of expression (10) to the array of $k_{\rm mask}$ values by minimizing the residual

$$\sum_{\bf s} [k_{\rm mask} - k_{\rm sol} \exp(-B_{\rm sol}\, s^2/4)]^2 \tag{31}$$

for all $k_{\rm mask} > 0$. This can be achieved analytically as described in Appendix *A*. Similarly, one can fit $k_{\rm overall} \exp(-B_{\rm overall}\, s^2/4)$ to the array of K values.

Equations (42), (43) and (45) in Section 2.4 of Afonine *et al.* (2013) are also updated as follows

$$\mathbf{b} = \left[\sum_{\bf s} I({\bf s}) I_1({\bf s}_1), \ldots, \sum_{\bf s} I({\bf s}) I_N({\bf s}_N), 1 \right]^t, \tag{42}$$

$$\mathrm{LS}(K, k_{\rm mask}) = \sum_{\bf s} \left\{ \left[\sum_{j=1}^{N} \alpha_j |\mathbf{F}_{\rm calc}({\bf s}_j) + k_{\rm mask} \mathbf{F}_{\rm mask}({\bf s}_j)|^2 \right] - K I_{\bf s} \right\}^2, \tag{43}$$

$$\mathrm{LS}(K, k_{\rm mask}) = \sum_{\bf s} \left[(k_{\rm mask}^2 w_{\bf s} + 2k_{\rm mask} v_{\bf s} + u_{\bf s}) - K I_{\bf s} \right]^2. \tag{45}$$

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