A new method for quantitative phase analysis using X-ray powder diffraction: direct derivation of weight fractions from observed integrated intensities and chemical compositions of individual phases. Corrigendum

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Erroneous equations in the paper by Toraya [*J. Appl. Cryst.* (2016), **49**, 1508–1516] are corrected.

In the paper by Toraya (2016), equations (9) and (10) on page 1511 were erroneously given. The correct equations are as follows:

For $k' = k$

$$\frac{\partial w_k}{\partial I_{jk}} = w_k(1 - w_k)G_{jk}\left(\sum_{j=1}^{N_k} I_{jk}G_{jk}\right)^{-1}.$$

For $k' \neq k$

$$\frac{\partial w_k}{\partial I_{jk'}} = -w_k w_{k'} G_{jk'}\left(\sum_{j=1}^{N_{k'}} I_{jk'}G_{jk'}\right)^{-1}. \tag{9}$$

$$\begin{aligned}
\text{s.u.}(w_k) = w_k\Bigg[&(1 - 2w_k)\left(\sum_{j=1}^{N_k} I_{jk}G_{jk}\right)^{-2} \sum_{j=1}^{N_k} G_{jk}^2\sigma^2(I_{jk}) \\
&+ \sum_{k'=1}^{K} w_{k'}^2\left(\sum_{j=1}^{N_{k'}} I_{jk'}G_{jk'}\right)^{-2} \sum_{j=1}^{N_{k'}} G_{jk'}^2\sigma^2(I_{jk'})\Bigg]^{1/2}. \tag{10}
\end{aligned}$$

The amounts of underestimation by the erroneous equations were in the range of 18–37% for individual test samples and 24% in grand average.

References

Toraya, H. (2016). *J. Appl. Cryst.* **49**, 1508–1516.