16 Data analysis

(1) Given three independent measurements of the lattice constant of a cubic crystal, 16.34 ± 0.31 Å, 16.19 ± 0.37 Å and 16.71 ± 0.11 Å, what is the best estimate of its value and the related 1σ uncertainty.

This question involves the application of the results derived in question (3) of the worked examples section of chapter 16 of the Foundations of Science Mathematics primer (2nd edition). Denoting the data by $\{d_k \pm \sigma_k\}$, where (in Å)

$$d_1 = 16.34\,, \quad d_2 = 16.19\,, \quad d_3 = 16.71$$
$$\sigma_1 = \ 0.31\,, \quad \sigma_2 = \ 0.37\,, \quad \sigma_3 = \ 0.11$$

the weights assigned to the measurements, $w_k = 1/\sigma_k^{\,2}$, become (in Å^{-2})

$$w_1 = 10.4\,, \quad w_2 = 7.3\,, \quad w_3 = 82.6$$

The best estimate of the lattice constant, and its uncertainty, is then given by the weighted mean

$$\sum_{k=1}^{3} w_k\, d_k \Bigg/ \sum_{k=1}^{3} w_k \ \pm \ \left(\sum_{k=1}^{3} w_k\right)^{-1/2} = \frac{1668}{100.3} \pm \frac{1}{\sqrt{100.3}} \text{ Å}$$
$$= \underline{16.63 \pm 0.10 \text{ Å}}$$

This is close to the largest measurement because its error-bar is smaller than those of the other two by a factor of around three (and, so, it carries a weight that is about ten times larger).

(2) The lattice constant of a cubic crystal, a, increases linearly with temperature, T, so that $a = mT + c$. Measurements at 20K, 50K and 80K, respectively, yield values of

$$16.032 \pm 0.027 \text{ Å}\,, \quad 16.249 \pm 0.013 \text{ Å} \quad \text{and} \quad 16.517 \pm 0.021 \text{ Å}$$

Evaluate the least-squares estimate of the expansion coefficient, m.

This question involves the application of the results derived in question (4) of the worked examples section of chapter 16 of the Foundations of Science Mathematics primer (2nd edition). Denoting the data by $\{d_k \pm \sigma_k\}$, where (in Å)

$$d_1 = 16.032\,, \quad d_2 = 16.249\,, \quad d_3 = 16.517$$
$$\sigma_1 = \ 0.027\,, \quad \sigma_2 = \ 0.013\,, \quad \sigma_3 = \ 0.021$$

corresponding to the measurements at temperatures (in K)

$$T_1 = 20\,, \quad T_2 = 50\,, \quad T_3 = 80$$

With $w_k = 1/\sigma_k^{\,2}$, so that (in Å^{-2})

$$w_1 = 1372\,, \quad w_2 = 5917\,, \quad w_3 = 2268$$

the data yield the following cogent parameters:

$$\alpha \ = \ \sum_{k=1}^{3} w_k\, T_k^2 \ = \ 2.985 \times 10^7 \ \mathrm{K}^2\,\text{Å}^{-2}$$

$$\beta \ = \ \sum_{k=1}^{3} w_k\, T_k \ = \ 5.047 \times 10^5 \ \mathrm{K}\,\text{Å}^{-2}$$

$$\mathrm{W} \ = \ \sum_{k=1}^{3} w_k \ = \ 9556\ \text{Å}^{-2}$$

$$\lambda \ = \ \sum_{k=1}^{3} w_k\, T_k\, d_k \ = \ 8.244 \times 10^6 \ \mathrm{K}\,\text{Å}^{-1}$$

$$\mu \ = \ \sum_{k=1}^{3} w_k\, d_k \ = \ 1.556 \times 10^5 \ \text{Å}^{-1}$$

Defining $\mathrm{D} = \alpha\,\mathrm{W} - \beta^2$, the least-squares estimate of the expansion coefficient is given by

$$m \ = \ \frac{\mathrm{W}\lambda - \beta\mu}{\mathrm{D}} \pm \sqrt{\frac{\mathrm{W}}{\mathrm{D}}} \ = \ \frac{2.483 \times 10^8}{3.052 \times 10^{10}} \ \pm \ \sqrt{\frac{9556}{3.052 \times 10^{10}}} \ \text{Å}\,\mathrm{K}^{-1}$$

$$= \ \underline{0.0082 \pm 0.0006\ \text{Å}\,\mathrm{K}^{-1}}$$