

3.2. THE LEAST-SQUARES PLANE

This is only an approximation, because the residuals $1 - \mathbf{b}^T \mathbf{r}$ are not the differences between the observations and appropriate linear functions of the parameters, nor are their variances (the $\mathbf{b}^T \mathbf{M} \mathbf{b}$'s) independent of the parameters (or, in turn, the errors in the observations).

We ask also about the perpendicular distances, e , of atoms to plane and the mean-square deviation $(\delta e)^2$ to be expected in e .

$$e = (1 - \mathbf{b}^T \mathbf{r}) / \sqrt{\mathbf{b}^T \mathbf{b}} = d(1 - \mathbf{b}^T \mathbf{r})$$

$$\delta e = -d(\mathbf{b}^T \boldsymbol{\eta} + \mathbf{r}^T \boldsymbol{\varepsilon}) + O(\eta^2).$$

Here $\boldsymbol{\eta}$ and $\boldsymbol{\varepsilon}$ are the errors in \mathbf{r} and \mathbf{b} . Neglecting ' $O(\eta^2)$ ' then leads to

$$\overline{(\delta e)^2} = d^2(\mathbf{b}^T \overline{\boldsymbol{\eta} \boldsymbol{\eta}^T} \mathbf{b} + 2\mathbf{b}^T \overline{\boldsymbol{\eta} \boldsymbol{\varepsilon}^T} \mathbf{r} + \mathbf{r}^T \overline{\boldsymbol{\varepsilon} \boldsymbol{\varepsilon}^T} \mathbf{r}).$$

We have $\overline{\boldsymbol{\eta} \boldsymbol{\eta}^T} = \mathbf{M} = \mathbf{P}^{-1}$, but $\overline{\boldsymbol{\eta} \boldsymbol{\varepsilon}^T}$ and $\overline{\boldsymbol{\varepsilon} \boldsymbol{\varepsilon}^T}$ perhaps still need to be evaluated.

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