University of São Paulo
São Carlos School of Engineering
Department of Aeronautical Engineering

Curve fitting – Part 2

Ricardo Afonso Angélico
raa@sc.usp.br

Linear curve fitting

$$\chi^2 = \sum_i \frac{(y_i - y(x_i))^2}{\alpha_i^2} \qquad y(x_i) = m\, x_i + c$$

$$c = \frac{\sum_i w_i x_i^2 \sum_i w_i y_i - \sum_i w_i x_i \sum_i w_i x_i y_i}{\Delta'} \qquad \alpha_m = \sqrt{\frac{\sum_i w_i}{\Delta'}}$$

$$m = \frac{\sum_i w_i \sum_i w_i x_i y_i - \sum_i w_i x_i \sum_i w_i y_i}{\Delta'} \qquad \alpha_c = \sqrt{\frac{\sum_i w_i x_i^2}{\Delta'}}$$

$$\Delta' = \sum_i w_i \sum_i w_i x_i^2 - \left(\sum_i w_i x_i\right)^2$$

Linear curve fitting

Fig. 6.2 Weighted (solid) and unweighted (dashed) lines of best fit for two of the data sets of Fig. 6.1 Details of the gradients, intercepts and their uncertainties can be found in Table 6.1.

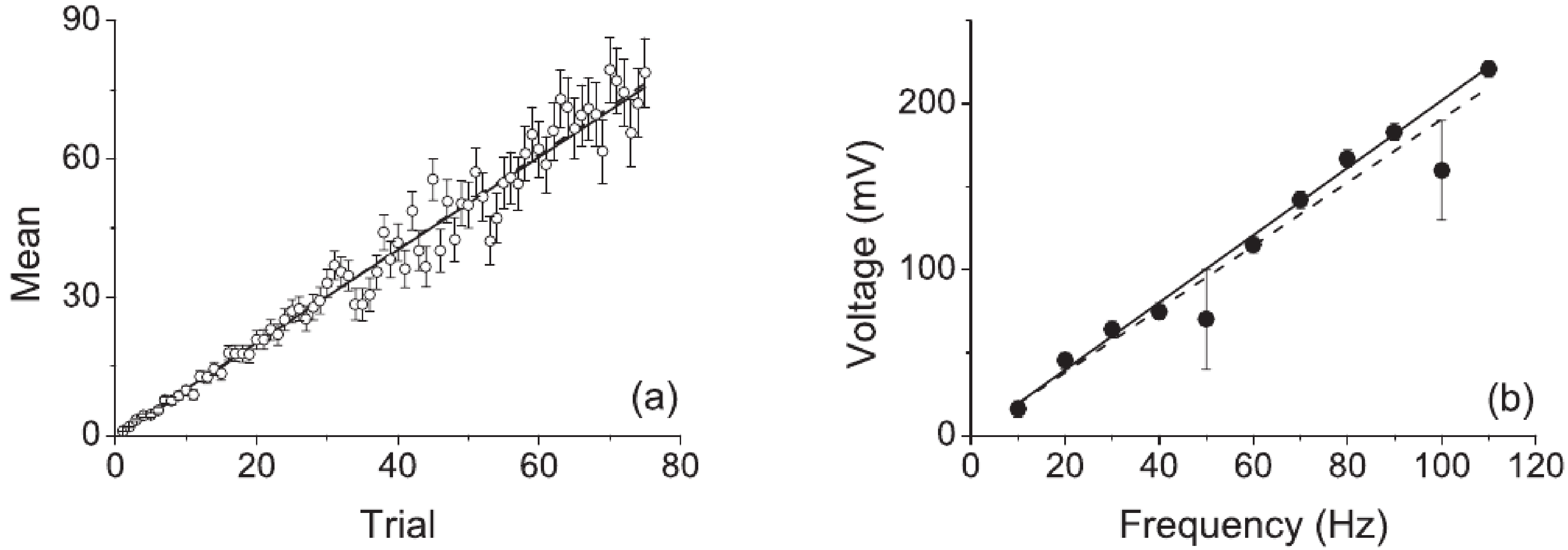
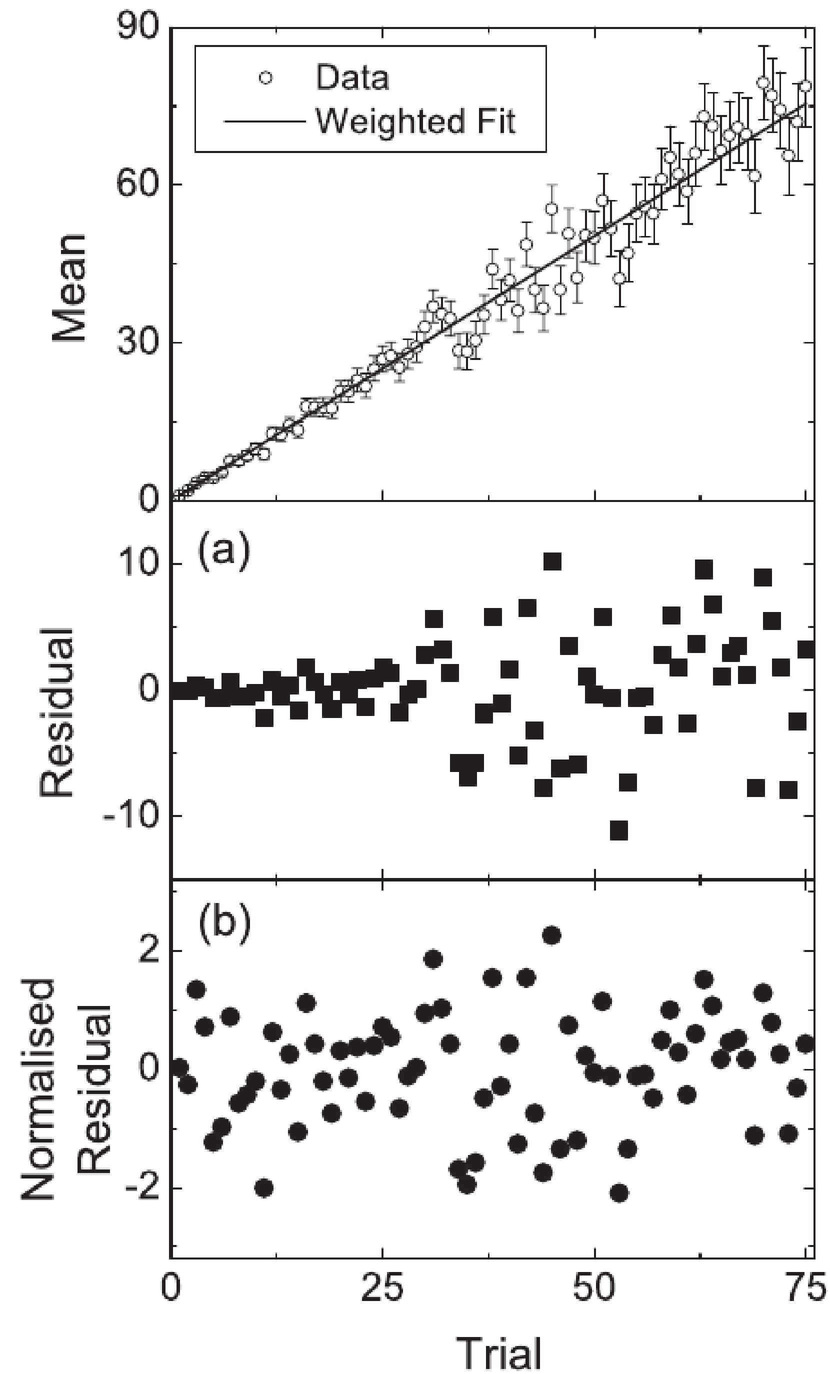


Table 6.1 Details of the gradients and intercepts from Fig. 6.2.

	Graph (a)		Graph (b)	
	Unweighted	Weighted	Unweighted	Weighted
Gradient	1.03 ± 0.02	1.01 ± 0.01	(1.9 ± 0.2) mV/Hz	(2.03 ± 0.05) mV/Hz
Intercept	-0.5 ± 0.9	0.01 ± 0.08	$(0 \pm 1) \times 10$ mV	(-1 ± 3) mV

Residual analysis

$$R_i = \frac{y_i - y(x_i)}{\alpha_i}$$



Error analysis

$$\chi^2(\overline{a}_j + \Delta a_j) = \chi^2(\overline{a}_j) + \frac{1}{2}\frac{\partial^2\chi^2}{\partial a_j^2}\bigg|_{\overline{a}_j}(\Delta a_j)^2 \qquad \alpha_j = \sqrt{\frac{2}{\left(\frac{\partial^2\chi^2}{\partial a_j^2}\right)}}$$

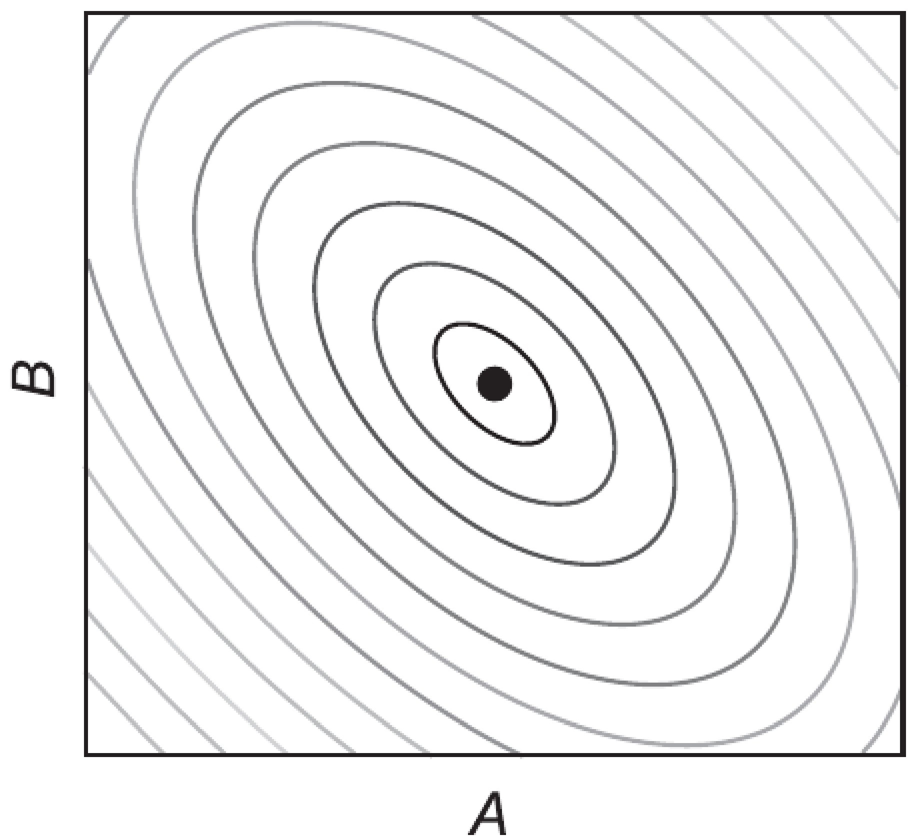


Fig. 6.6 Contours of constant χ^2 in the $A-B$ plane for a general two-parameter nonlinear function $f(A, B)$. The minimum value of χ^2, $\chi^2_{\min}$, is obtained with the best-fit values of the parameters, $\overline{A}$ and $\overline{B}$, shown by the dot in the centre. The contours increase in magnitude as one departs from the best-fit parameters.

Error analysis

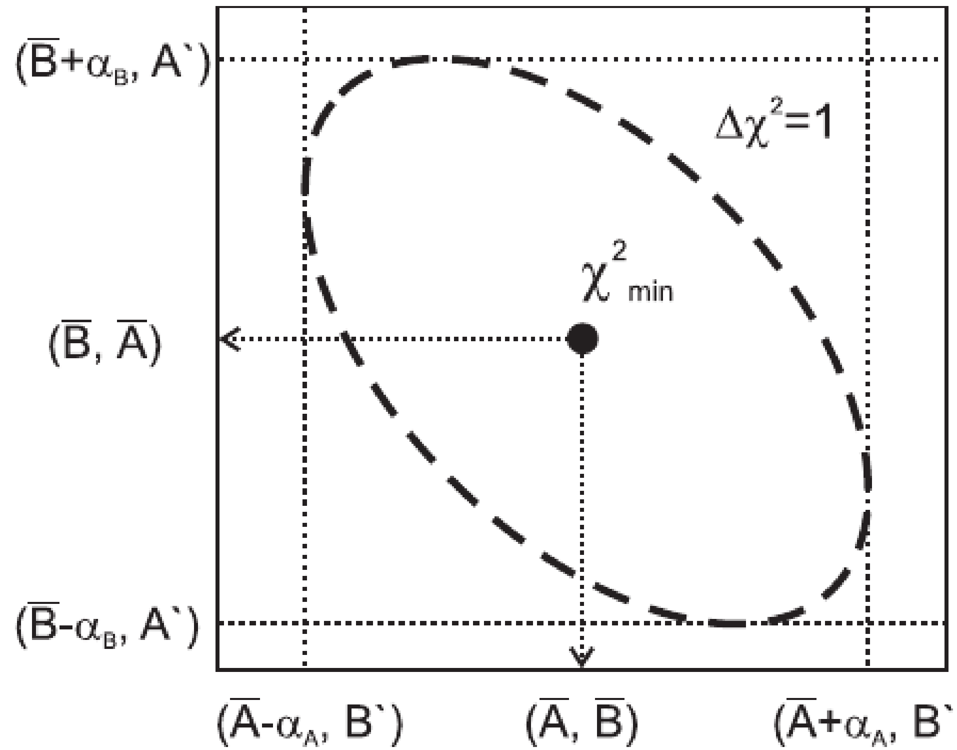
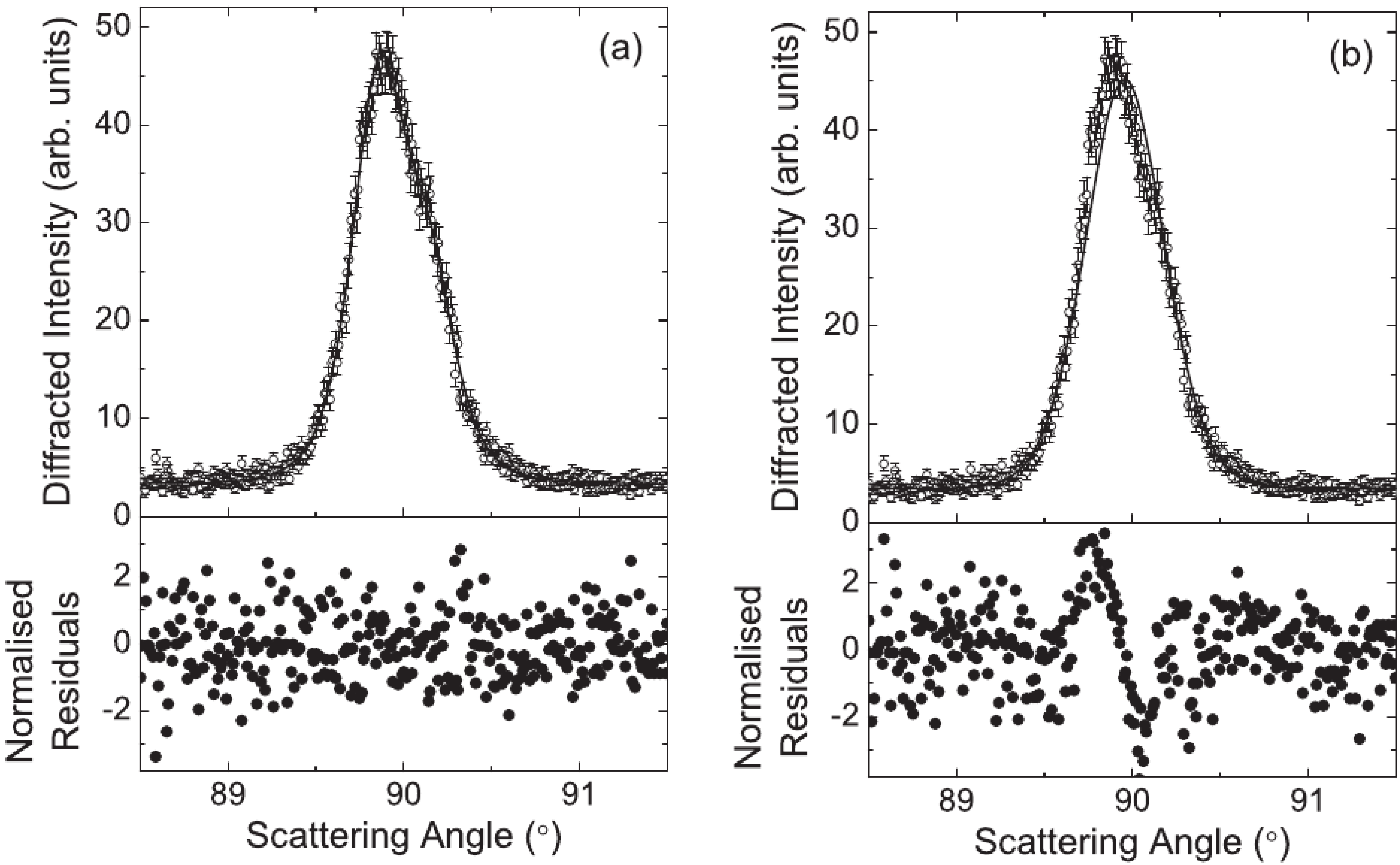


Fig. 6.7 The $\Delta\chi^2 = 1$ contour in the A–B plane. The horizontal and vertical tangent planes define the uncertainties in the parameters.

Table 6.2 Confidence limits associated with various $\Delta\chi^2$ contours for one degree of freedom.

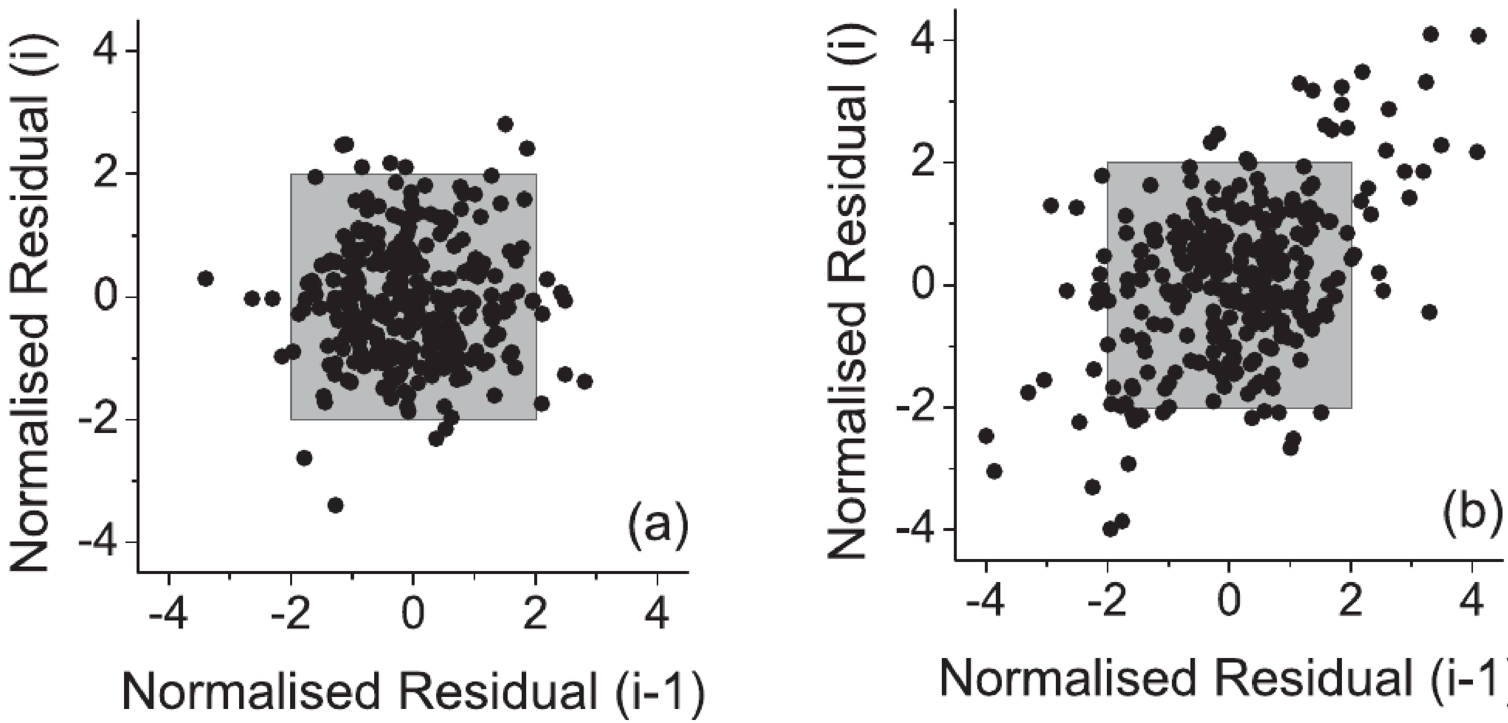
$\Delta\chi^2$ contour	1.00	2.71	4.00	6.63	9.00
Measurements within range	68.3% 1σ	90.0%	95.4% 2σ	99.0%	99.7% 3σ

Testing the fit using residuals



D test

$$\mathcal{D} = \frac{\sum_{i=2}^{N} [R_i - R_{i-1}]^2}{\sum_{i=1}^{N} [R_i]^2}$$



(1) $\mathcal{D} = 0$: systematically correlated residuals;
(2) $\mathcal{D} = 2$: randomly distributed residuals that follow a Gaussian distribution;
(3) $\mathcal{D} = 4$: systematically anticorrelated residuals.

Covariance and correlation

$$=1 \ \frac{\partial \chi^2}{\partial a_j}\bigg|_{\mathbf{a}_s} \Delta a_j \qquad \overset{N}{} R_i^2 \qquad R_i = \frac{y_i - y(x_i;\mathbf{a})}{\alpha_i} \qquad \frac{\partial^2 \chi^2}{\partial a_j \partial a_k}$$

$$\mathbf{h}) \approx \chi^2(\mathbf{a}_s) + \mathbf{g}_s^{\mathrm{T}}\mathbf{h} + \frac{1}{2}\mathbf{h}^{\mathrm{T}}\mathbf{H}_s\mathbf{h}$$

$$\mathbf{g}_s = \nabla \chi^2(\mathbf{a}_s) = \left[\frac{\partial \chi^2}{\partial a_1}, \cdots, \frac{\partial \chi^2}{\partial a_{\mathcal{N}}}\right]^{\mathrm{T}} \qquad \mathbf{J}_s = \mathbf{J}(\mathbf{a}_s) = \begin{bmatrix} \frac{\partial R_1}{\partial a_1} & \cdots & \frac{\partial R_1}{\partial a_{\mathcal{N}}} \\ \vdots & \ddots & \vdots \\ \frac{\partial R_N}{\partial a_1} & \cdots & \frac{\partial R_N}{\partial a_{\mathcal{N}}} \end{bmatrix}$$

$$\mathbf{H}_s = \mathbf{H}(\mathbf{a}_s) = \begin{bmatrix} \frac{\partial^2 \chi^2}{\partial a_1^2} & \cdots & \frac{\partial^2 \chi^2}{\partial a_1 \partial a_{\mathcal{N}}} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 \chi^2}{\partial a_1 \partial a_{\mathcal{N}}} & \cdots & \frac{\partial^2 \chi^2}{\partial a_{\mathcal{N}}^2} \end{bmatrix}$$

Covariance and correlation

$$\chi^2 = \sum_{i=1}^{N} R_i^2 \qquad R_i = \frac{y_i - y\left(x_i; \mathsf{a}\right)}{\alpha_i}$$

$$\chi^2\left(\mathsf{a}_s + \mathsf{h}\right) \approx \chi^2\left(\mathsf{a}_s\right) + \sum_{j=1}^{\mathcal{N}} \left.\frac{\partial \chi^2}{\partial a_j}\right|_{\mathsf{a}_s} \Delta a_j$$

$$+\frac{1}{2} \sum_{j=1}^{\mathcal{N}} \left.\frac{\partial^2 \chi^2}{\partial a_j^2}\right|_{\mathsf{a}_s} \left(\Delta a_j\right)^2 .$$

$$\chi^2\left(\mathsf{a}_s + \mathsf{h}\right) \approx \chi^2\left(\mathsf{a}_s\right) + \mathsf{g}_s^{\mathrm{T}}\mathsf{h} + \frac{1}{2}\mathsf{h}^{\mathrm{T}}\mathsf{H}_s\mathsf{h}$$

$$\frac{\partial^2 \chi^2}{\partial a_j \partial a_k} = \frac{\partial^2}{\partial a_j \partial a_k} \sum_i R_i^2 = 2 \sum_i \frac{\partial R_i}{\partial a_j} \frac{\partial R_i}{\partial a_k} + 2 \sum_i R_i \frac{\partial^2 R_i}{\partial a_j \partial a_k}$$

Covariance and correlation matrices

$$\chi^2(\mathbf{a}_s+\mathbf{h}) \approx \chi^2(\mathbf{a}_s) + \sum_{j=1}^{\mathcal{N}} \left.\frac{\partial \chi^2}{\partial a_j}\right|_{\mathbf{a}_s} \Delta a_j$$

$$+\frac{1}{2}\sum_{j=1}^{\mathcal{N}} \left.\frac{\partial^2 \chi^2}{\partial a_j^2}\right|_{\mathbf{a}_s} (\Delta a_j)^2 .$$

$$\frac{\partial^2 \chi^2}{\partial a_j \partial a_k} = \frac{\partial^2}{\partial a_j \partial a_k}\sum_i R_i^2 = 2\sum_i \frac{\partial R_i}{\partial a_j}\frac{\partial R_i}{\partial a_k} + 2\sum_i R_i \frac{\partial^2 R_i}{\partial a_j \partial a_k}$$

$$\mathbf{J}_s = \mathbf{J}(\mathbf{a}_s) = \begin{bmatrix} \frac{\partial R_1}{\partial a_1} & \cdots & \frac{\partial R_1}{\partial a_{\mathcal{N}}} \\ \vdots & \ddots & \vdots \\ \frac{\partial R_N}{\partial a_1} & \cdots & \frac{\partial R_N}{\partial a_{\mathcal{N}}} \end{bmatrix} \quad \mathbf{H}_s = \mathbf{H}(\mathbf{a}_s) = \begin{bmatrix} \frac{\partial^2 \chi^2}{\partial a_1^2} & \cdots & \frac{\partial^2 \chi^2}{\partial a_1 \partial a_{\mathcal{N}}} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 \chi^2}{\partial a_1 \partial a_{\mathcal{N}}} & \cdots & \frac{\partial^2 \chi^2}{\partial a_{\mathcal{N}}^2} \end{bmatrix}$$

$$\mathbf{H} \approx 2\mathbf{J}^{\mathrm{T}}\mathbf{J}$$

Covariance and correlation matrices

$$\chi^2(\mathrm{a}_s + \mathrm{h}) \approx \chi^2(\mathrm{a}_s) + \sum_{j=1}^{\mathcal{N}} \left.\frac{\partial \chi^2}{\partial a_j}\right|_{\mathrm{a}_s} \Delta a_j$$

$$+\frac{1}{2}\sum_{j=1}^{\mathcal{N}} \left.\frac{\partial^2 \chi^2}{\partial a_j^2}\right|_{\mathrm{a}_s} (\Delta a_j)^2 .$$

$$\mathrm{J}_s = \mathrm{J}(\mathrm{a}_s) = \begin{bmatrix} \frac{\partial R_1}{\partial a_1} & \cdots & \frac{\partial R_1}{\partial a_{\mathcal{N}}} \\ \vdots & \ddots & \vdots \\ \frac{\partial R_N}{\partial a_1} & \cdots & \frac{\partial R_N}{\partial a_{\mathcal{N}}} \end{bmatrix} \quad \mathrm{H}_s = \mathrm{H}(\mathrm{a}_s) = \begin{bmatrix} \frac{\partial^2 \chi^2}{\partial a_1^2} & \cdots & \frac{\partial^2 \chi^2}{\partial a_1 \partial a_{\mathcal{N}}} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 \chi^2}{\partial a_1 \partial a_{\mathcal{N}}} & \cdots & \frac{\partial^2 \chi^2}{\partial a_{\mathcal{N}}^2} \end{bmatrix}$$

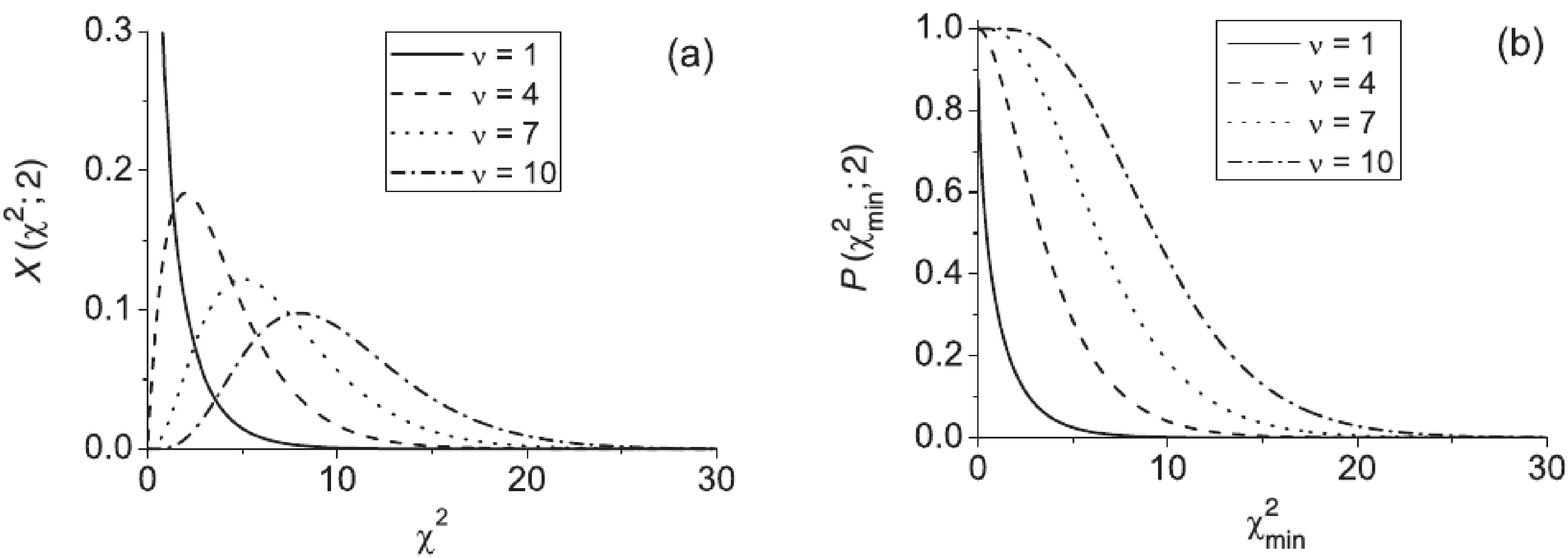
$$\boxed{\mathrm{H} \approx 2\mathrm{J}^{\mathrm{T}}\mathrm{J}}$$

$$[\,\mathrm{C}\,] = [\,\mathrm{A}\,]^{-1} \qquad \alpha_j = \sqrt{C_{jj}} \qquad \rho_{AB} = \frac{\sigma_{AB}}{\sigma_A \sigma_B} = \frac{C_{AB}}{\sqrt{C_{AA} C_{BB}}}$$

Testing the fit

$$X\left(\chi^2;\nu\right) = \frac{\left(\chi^2\right)^{\left(\frac{\nu}{2}-1\right)}\ \exp\left[-\chi^2/2\right]}{2^{\nu/2}\ \Gamma\left(\nu/2\right)} \qquad \nu = N - \mathcal{N}.$$

$$P\left(\chi^2_{\min} \le \chi^2 \le \infty;\nu\right) = \int_{\chi^2_{\min}}^{\infty} X\left(\chi^2;\nu\right)\ \mathrm{d}\chi^2.$$



Testing the fit

$$T = 2\pi\sqrt{\frac{L}{g}}\left[1 + \frac{1}{16}(\theta_{\max})^2\right]$$

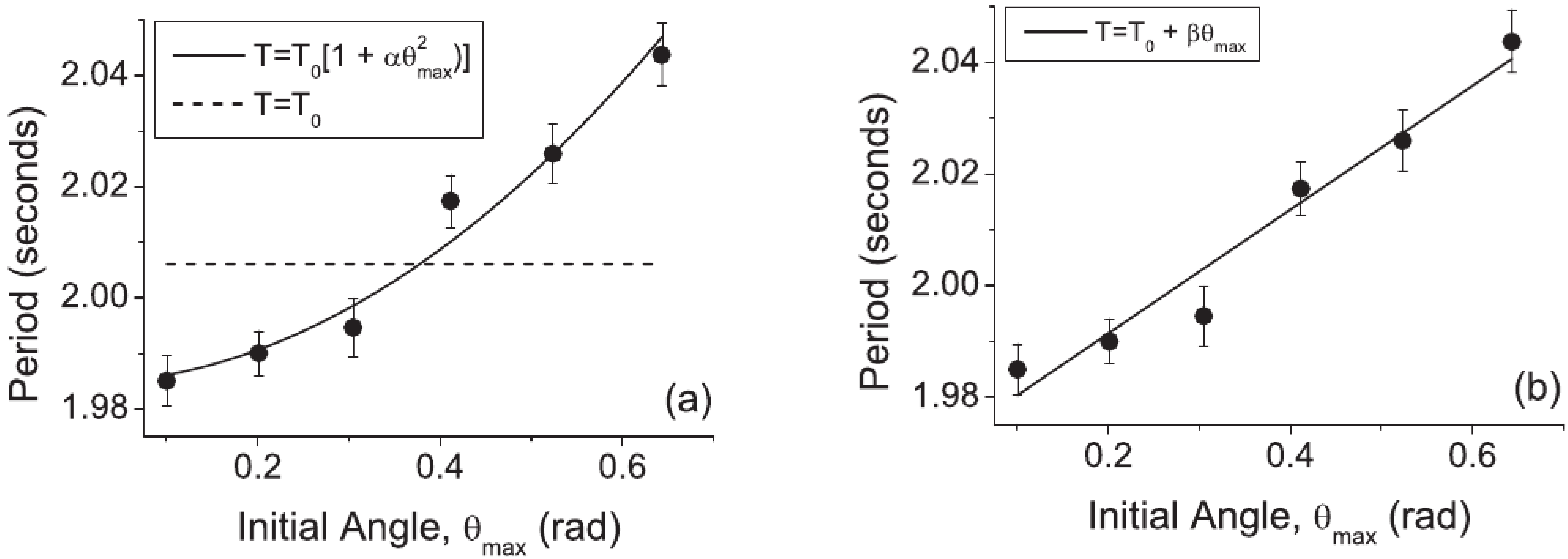


Table 8.2 Three different models are used for the dependence of the period of oscillation of a pendulum on the initial angular displacement.

Model	Degrees of freedom	$\chi^2_{\min}$	χ^2_ν	$P(\chi^2_{\min};\nu)$
$T = T_0$	5	107.2	21.4	1.6×10^{-21}
$T = T_0\left[1 + \alpha\,\theta^2_{\max}\right]$	4	3.39	0.9	0.49
$T = T_0\left[1 + \beta\,\theta_{\max}\right]$	4	4.39	1.1	0.36

I want to know more...