Least Square Straight Line Fit

$$\sum_{i=1}^{N}\frac{1}{\sigma_i^2}=\frac{1}{0.1^2}+\frac{1}{0.2^2}+\frac{1}{0.3^2}+\frac{1}{0.4^2}=142.36$$

$$\sum_{i=1}^{N}\frac{x_i}{\sigma_i^2}=\frac{0}{0.1^2}+\frac{1}{0.2^2}+\frac{2}{0.3^2}+\frac{3}{0.4^2}=65.97$$

$$\sum_{i=1}^{N}\frac{x_i^2}{\sigma_i^2}=\frac{0^2}{0.1^2}+\frac{1^2}{0.2^2}+\frac{2^2}{0.3^2}+\frac{3^2}{0.4^2}=125.69$$

$$\sum_{i=1}^{N}\frac{y_i}{\sigma_i^2}=\frac{-0.153}{0.1^2}+\frac{1.107}{0.2^2}+\frac{1.879}{0.3^2}+\frac{3.174}{0.4^2}=53.09$$

$$\sum_{i=1}^{N}\frac{y_i x_i}{\sigma_i^2}=\frac{0(-0.153)}{0.1^2}+\frac{1(1.107)}{0.2^2}+\frac{2(1.879)}{0.3^2}+\frac{3(3.174)}{0.4^2}=128.94$$

data

x	y	σ_y
0.0	-0.153	0.1
1.0	1.107	0.2
2.0	1.879	0.3
3.0	3.174	0.4

$$\mathrm{a}=\frac{\left(\sum_{i=1}^{N}\frac{1}{\sigma_i^2}\sum_{i=1}^{N}\frac{y_i x_i}{\sigma_i^2}-\sum_{i=1}^{N}\frac{x_i}{\sigma_i^2}\sum_{i=1}^{N}\frac{y_i}{\sigma_i^2}\right)}{\left(\sum_{i=1}^{N}\frac{1}{\sigma_i^2}\sum_{i=1}^{N}\frac{x_i^2}{\sigma_i^2}-\sum_{i=1}^{N}\frac{x_i}{\sigma_i^2}\sum_{i=1}^{N}\frac{x_i}{\sigma_i^2}\right)}=\frac{(141.36(128.94)-65.97(53.09))}{((142.36(125.69)-65.97^2)}=1.096910$$

$$\mathrm{b}=\frac{\left(\sum_{i=1}^{N}\frac{x_i^2}{\sigma_i^2}\sum_{i=1}^{N}\frac{y_i}{\sigma_i^2}-\sum_{i=1}^{N}\frac{x_i}{\sigma_i^2}\sum_{i=1}^{N}\frac{y_i x_i}{\sigma_i^2}\right)}{\left(\sum_{i=1}^{N}\frac{1}{\sigma_i^2}\sum_{i=1}^{N}\frac{x_i^2}{\sigma_i^2}-\sum_{i=1}^{N}\frac{x_i}{\sigma_i^2}\sum_{i=1}^{N}\frac{x_i}{\sigma_i^2}\right)}=\frac{(125.60(53.09)-65.97(128.94))}{((142.36(125.69)-65.97^2)}=\text{-}0.135397$$

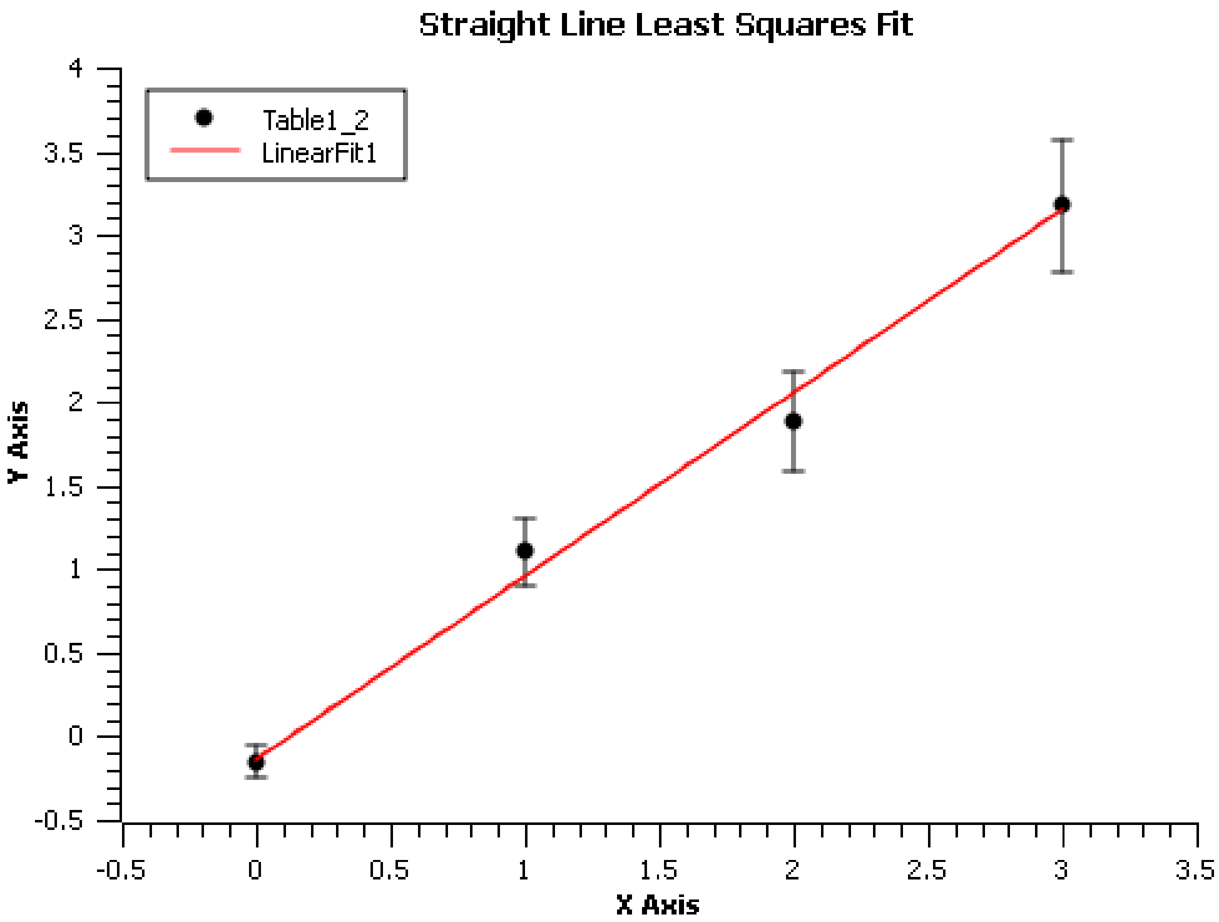
$$R^{-1} = \begin{vmatrix} \frac{1}{2}\frac{\partial^2 \chi^2}{\partial a \partial a} & \frac{1}{2}\frac{\partial^2 \chi^2}{\partial a \partial b} \\ \frac{1}{2}\frac{\partial^2 \chi^2}{\partial b \partial a} & \frac{1}{2}\frac{\partial^2 \chi^2}{\partial b \partial b} \end{vmatrix} = \begin{vmatrix} \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} & \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \\ \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} & \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \end{vmatrix} = \begin{vmatrix} 125.69 & 65.97 \\ 65.97 & 142.36 \end{vmatrix}$$

$$R = \begin{vmatrix} \sigma_{aa}^2 & \sigma_{ab}^2 \\ \sigma_{ba}^2 & \sigma_{bb}^2 \end{vmatrix} = \begin{vmatrix} \dfrac{\sum_{i=1}^{N} \frac{1}{\sigma_i^2}}{\left(\sum_{i=1}^{N} \frac{1}{\sigma_i^2} \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} - \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \right)} & \dfrac{-\sum_{i=1}^{N} \frac{x_i}{\sigma_i^2}}{\left(\sum_{i=1}^{N} \frac{1}{\sigma_i^2} \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} - \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \right)} \\ \dfrac{-\sum_{i=1}^{N} \frac{x_i}{\sigma_i^2}}{\left(\sum_{i=1}^{N} \frac{1}{\sigma_i^2} \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} - \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \right)} & \dfrac{\sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2}}{\left(\sum_{i=1}^{N} \frac{1}{\sigma_i^2} \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} - \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} \right)} \end{vmatrix} = \begin{vmatrix} 0.01051 & -0.004872 \\ -0.004872 & 0.009282 \end{vmatrix}$$

$$\sigma_a = 0.1025$$

$$\sigma_b = 0.0963$$

SciDavis line fit agrees with all these numbers to > 6 decimal places



$$\chi^2_{\text{minimum}} = 0.920 \;\; \text{for 2 D.O.F}$$

C.L. 63.1% trials would have a worse χ^2

SciDavis quotes the results as

b= -0.135 +/- 0.096

a = 1.10 +/- 0.10

This is commonly done but is wrong if a and b are highly correlated!

Let's plot the 2-D error contours for a and b
There are two ways to do this:

1) Plot $\Delta\chi^2$ contours in a and b

$$\Delta\chi^2 = \chi^2 - \chi^2_{\min} = \frac{(-0.153 - a\cdot 0.0 - b)^2}{0.1^2} + \frac{(1.107 - a\cdot 1.0 - b)^2}{0.2^2} + \frac{(1.879 - a\cdot 2.0 - b)^2}{0.3^2} + \frac{(3.174 - a\cdot 3.0 - b)^2}{0.4^2} - 0.920022$$

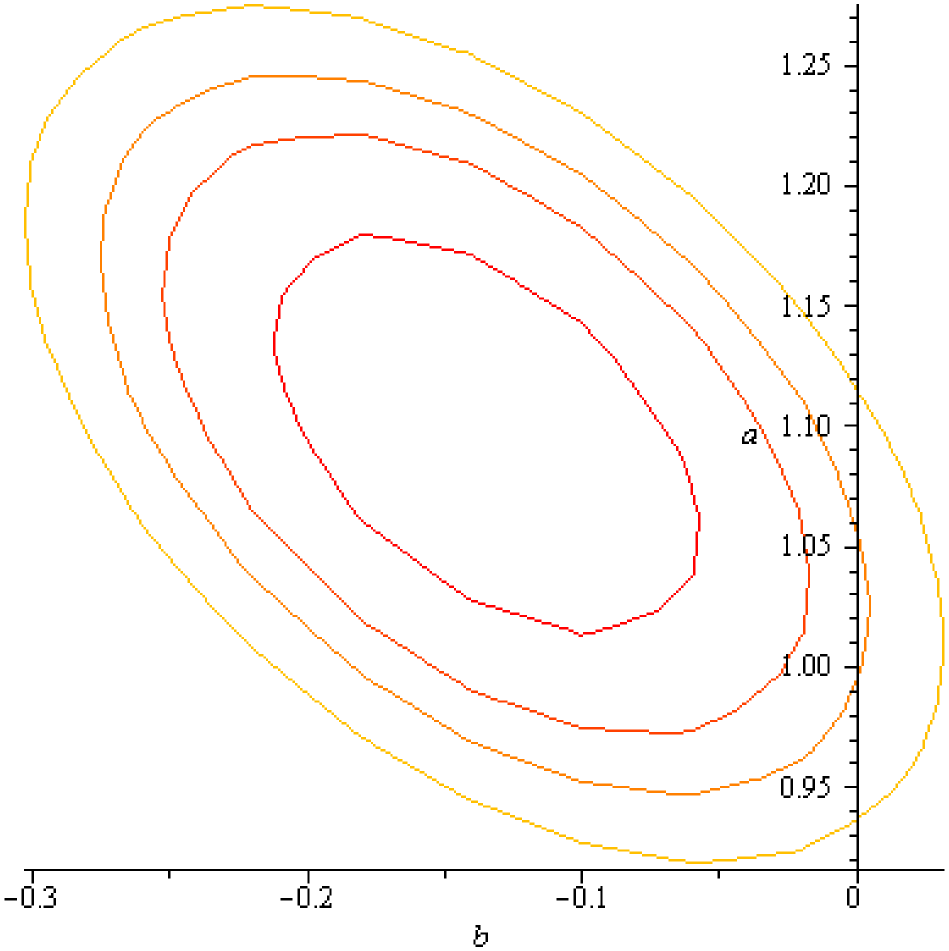
2) Plot error ellipse contours for a and b

$$\Delta\chi^2 = R^{-1}_{aa}a^2 + R^{-1}_{bb}b^2 + 2R^{-1}_{ab}ab$$

Shifting ellipse to center it on best fit a and b we get

$$\Delta\chi^2 = 125.69(a - 1.0969)^2 + 142.35(b + 0.13534)^2 + 2(65.972)(a - 1.0969)(b + 0.13534)$$

Note: both methods give identical ellipses



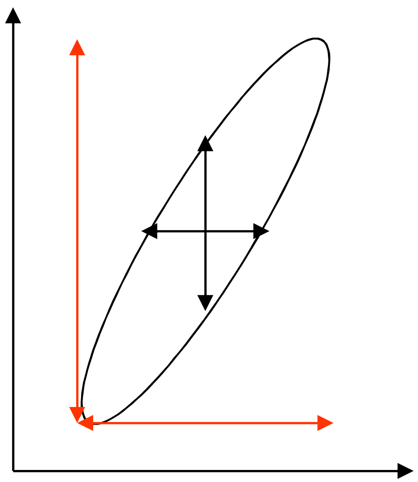
$\Delta\chi^2$ Confidence Levels

C.L.	1-D	2-D
20%	0.253	0.668
68%	1.00	1.51
90%	1.64	2.15
99%	2.58	3.03

$$\int_{-1}^{1} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} dx = 0.68$$

$$\int_{0}^{1.52} r e^{-\frac{r^2}{2}} dr = 0.68$$

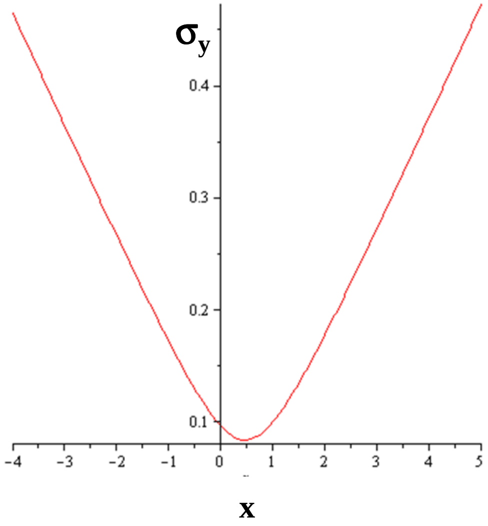
Contours containing 20%, 69%, 90% and 99% of random trials in 2-D



SciDavis Errors on single variable
Real Errors on single variable

If correlation large one must find the max min of each axis of the ellipse!

Extrapolation: What is the uncertainty in y at x=6?



$$y = a * x + b$$

$$\sigma_y^2 = \left(\frac{\partial y}{\partial a}\right)^2 \sigma_a^2 + \left(\frac{\partial y}{\partial b}\right)^2 \sigma_b^2 + 2\left(\frac{\partial y}{\partial a}\right)\left(\frac{\partial y}{\partial b}\right)\sigma_{ab} = \sigma_a^2 x^2 + \sigma_b^2 + 2\sigma_{ab} x$$

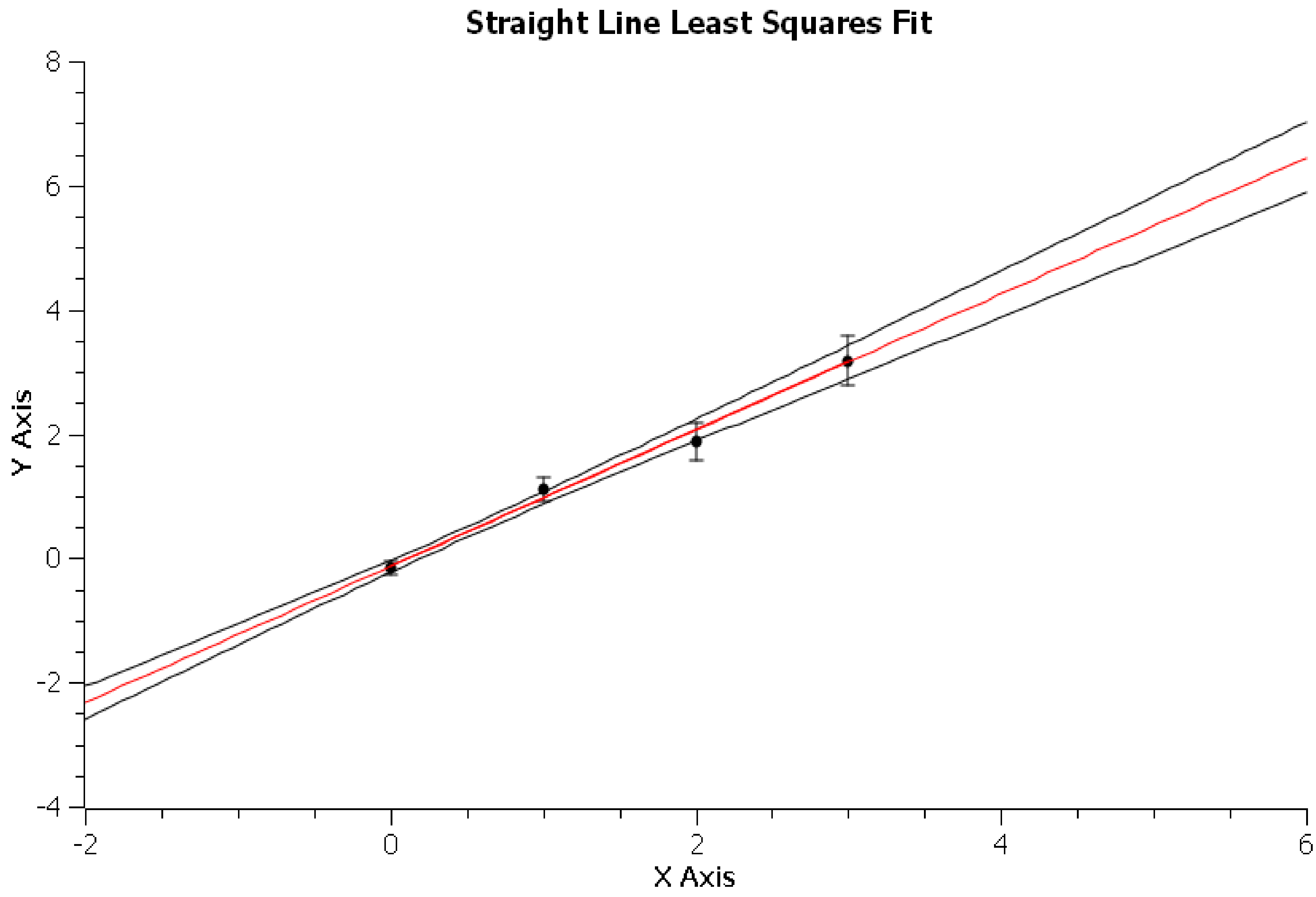
$$\sigma_y^2 = 0.01051 \cdot x^2 + 0.009282 + 2 \cdot -0.004872 * x =$$

$$0.01051 \cdot 6^2 + 0.009282 + 2 \cdot -0.004872 * 6 = 0.329$$

Note: The minimum of σ_y^2 is $\bar{x} = \frac{\sum_i \frac{x_i}{\sigma_i^2}}{\sum_i \frac{1}{\sigma_i^2}} = 0.4634$

Thus if one fits $y = a(x - \bar{x}) + b$ then σ_{ab}^2 would be zero!

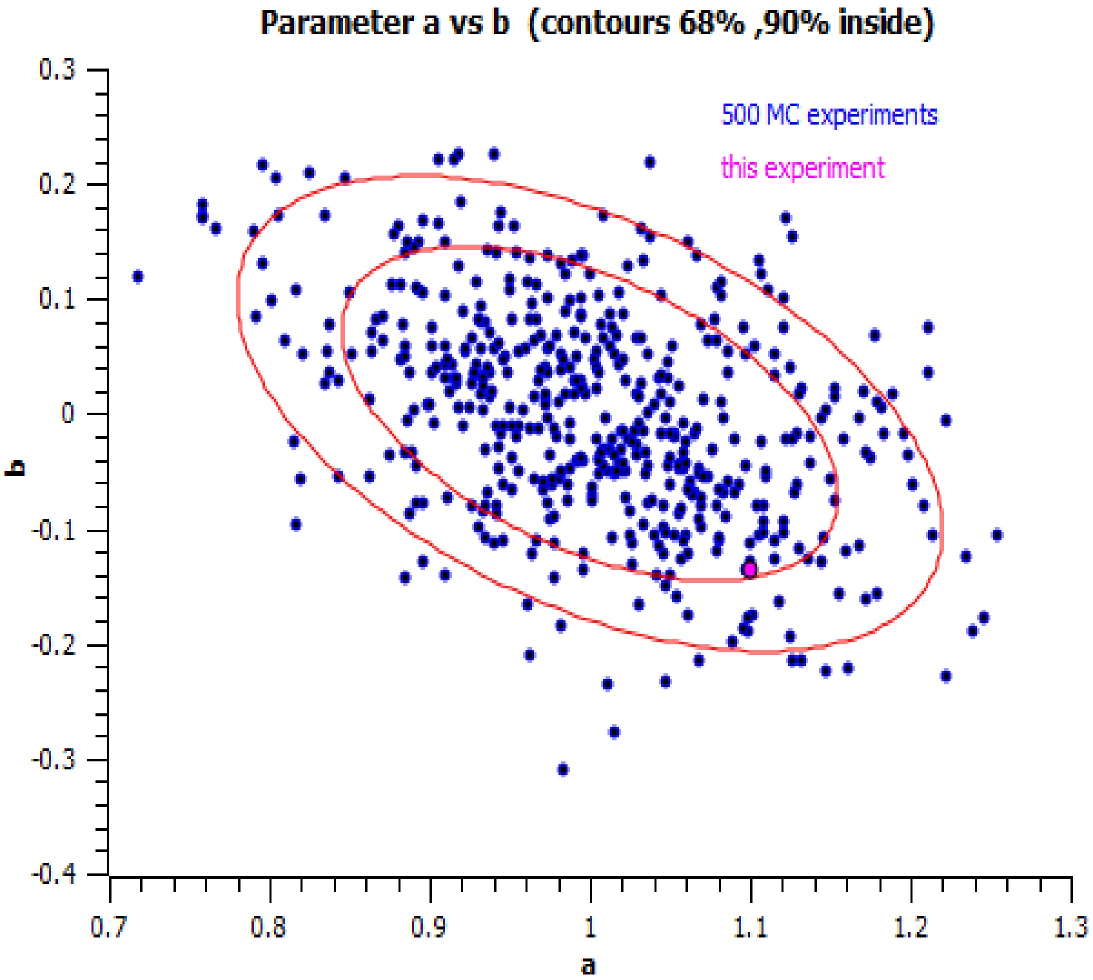
Extrapolation Uncertainty ±1σ



Repeat MC Experiment 100K Times to Test Statistics Predictions

Calculated Covariance Matrix $R = \begin{vmatrix} 0.0105 & -0.0049 \\ -0.0049 & 0.0093 \end{vmatrix}$ same as χ^2 prediction

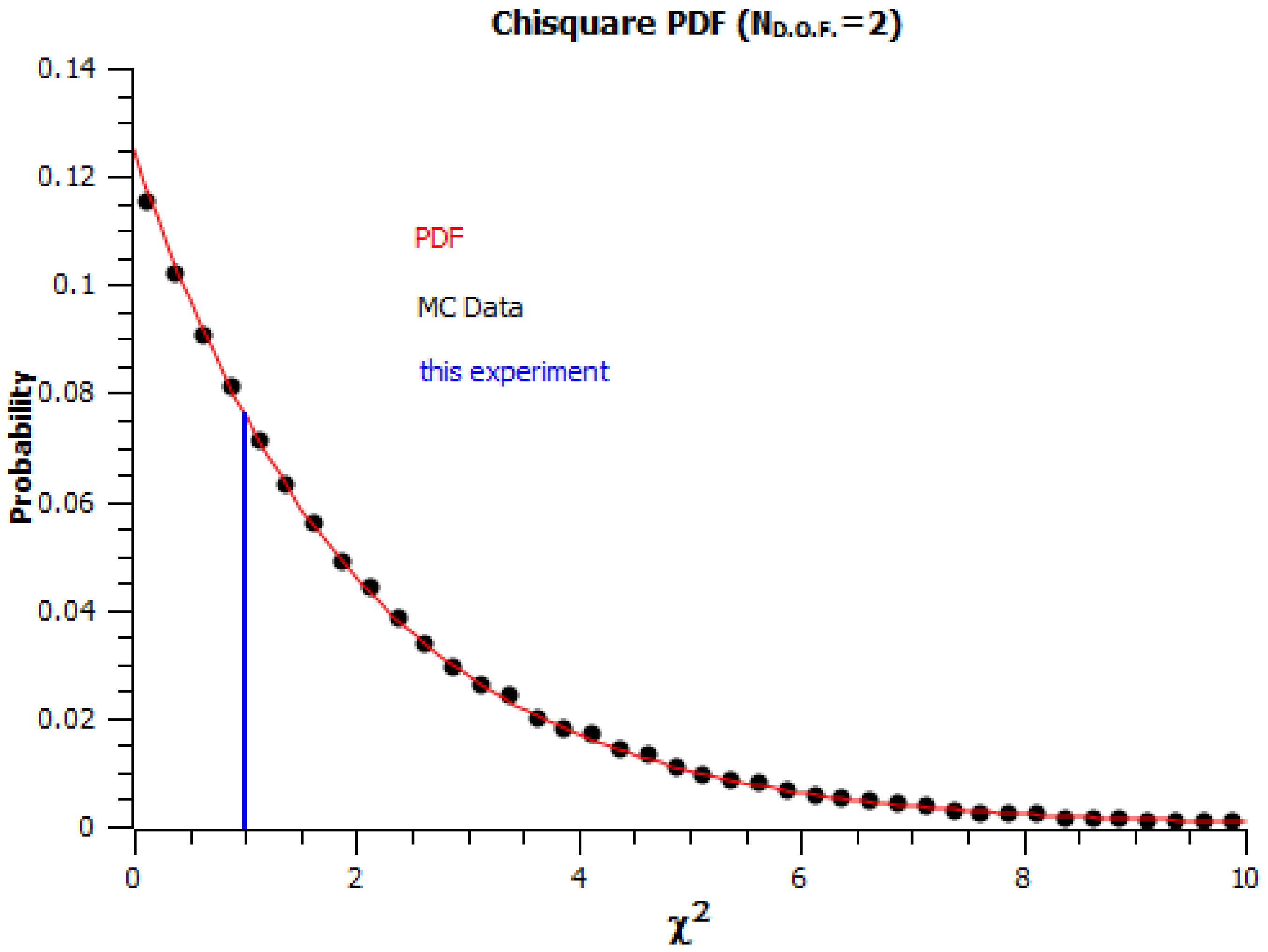
C.L. for "this experiment" 43.7%

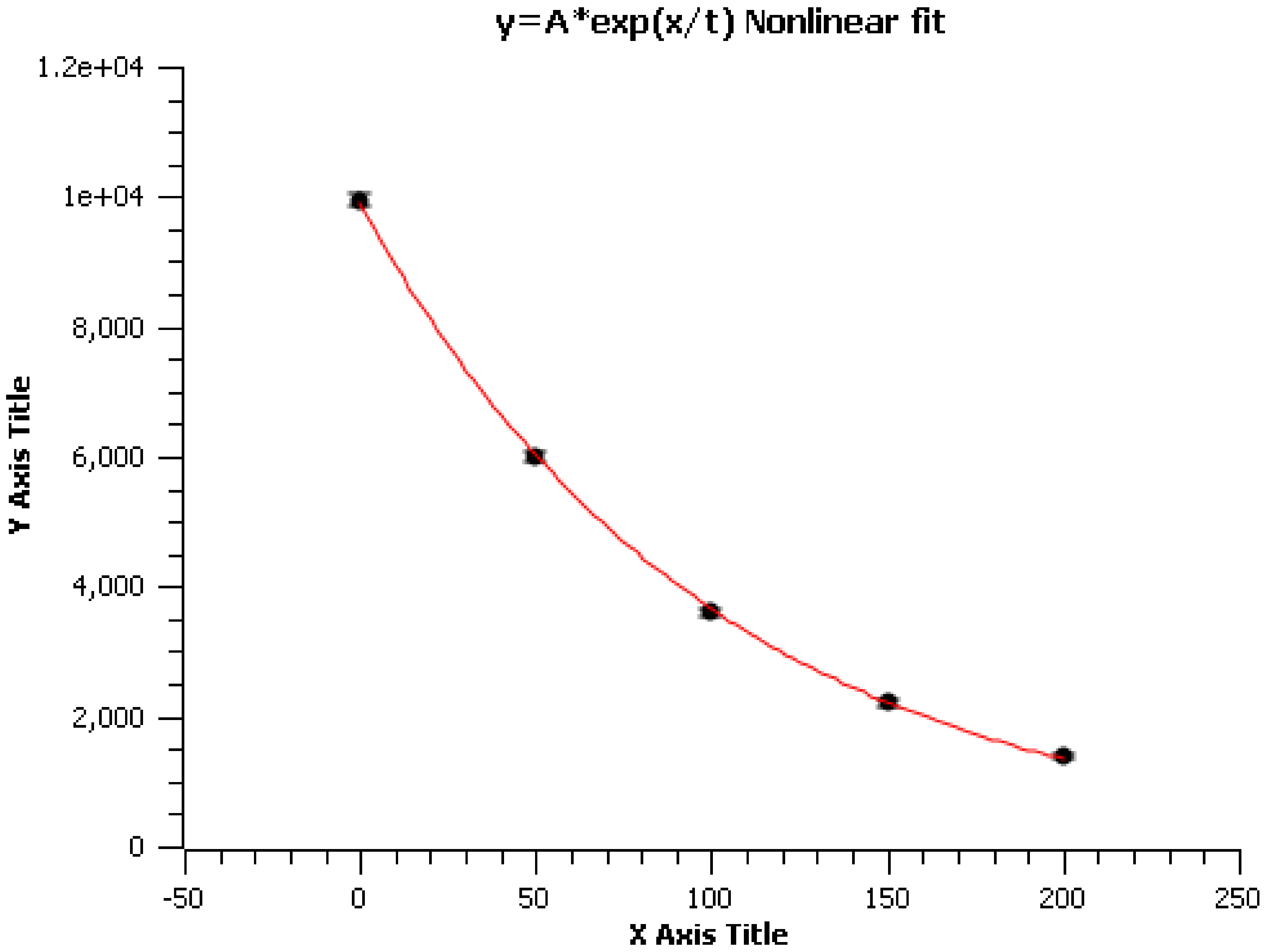


inside 68% ellypse 67,733/100,000
Inside 90% ellypse 90,106/100,000

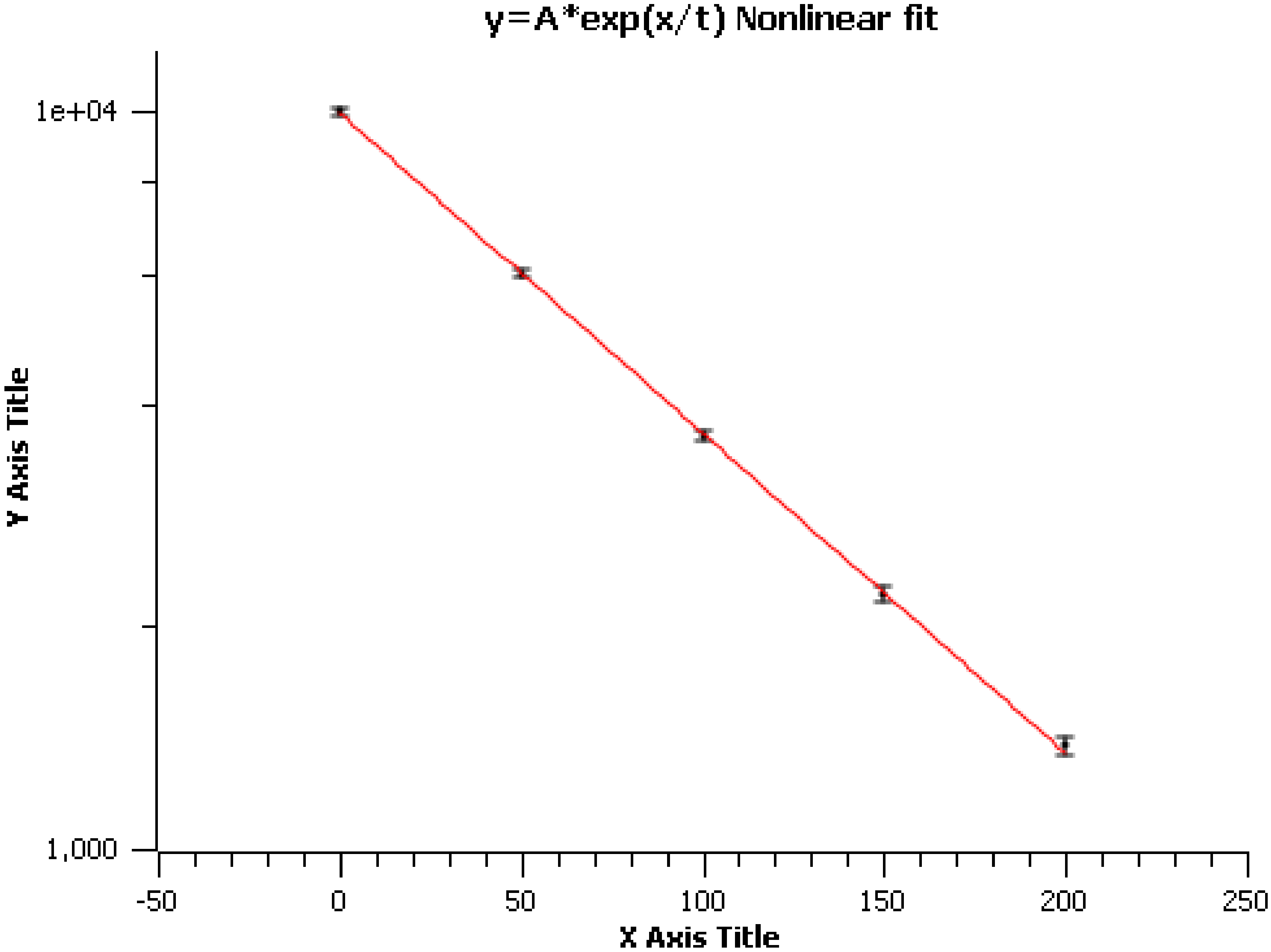
Repeat MC Experiment 100K Times to Test Statistics Predictions

63537/100000 of MC experiments have worse Chi-Square
C.L. predicted 63.1%





y=A*exp(x/t) Nonlinear fit
1.2e+04
1e+04
8,000
6,000
4,000
2,000
0
Y Axis Title
-50
0
50
100
150
200
250
X Axis Title


y=A*exp(x/t) Nonlinear fit
1e+04
1,000
Y Axis Title
-50
0
50
100
150
200
250
X Axis Title