Lecture 4: some topics in extrapolation

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- Theory/formalism to extrapolate data (e.g. R matrix)

  Example: $^{12}C(\alpha,\gamma)^{16}O$ in helium burning

known potential, Φ known

unknown potential

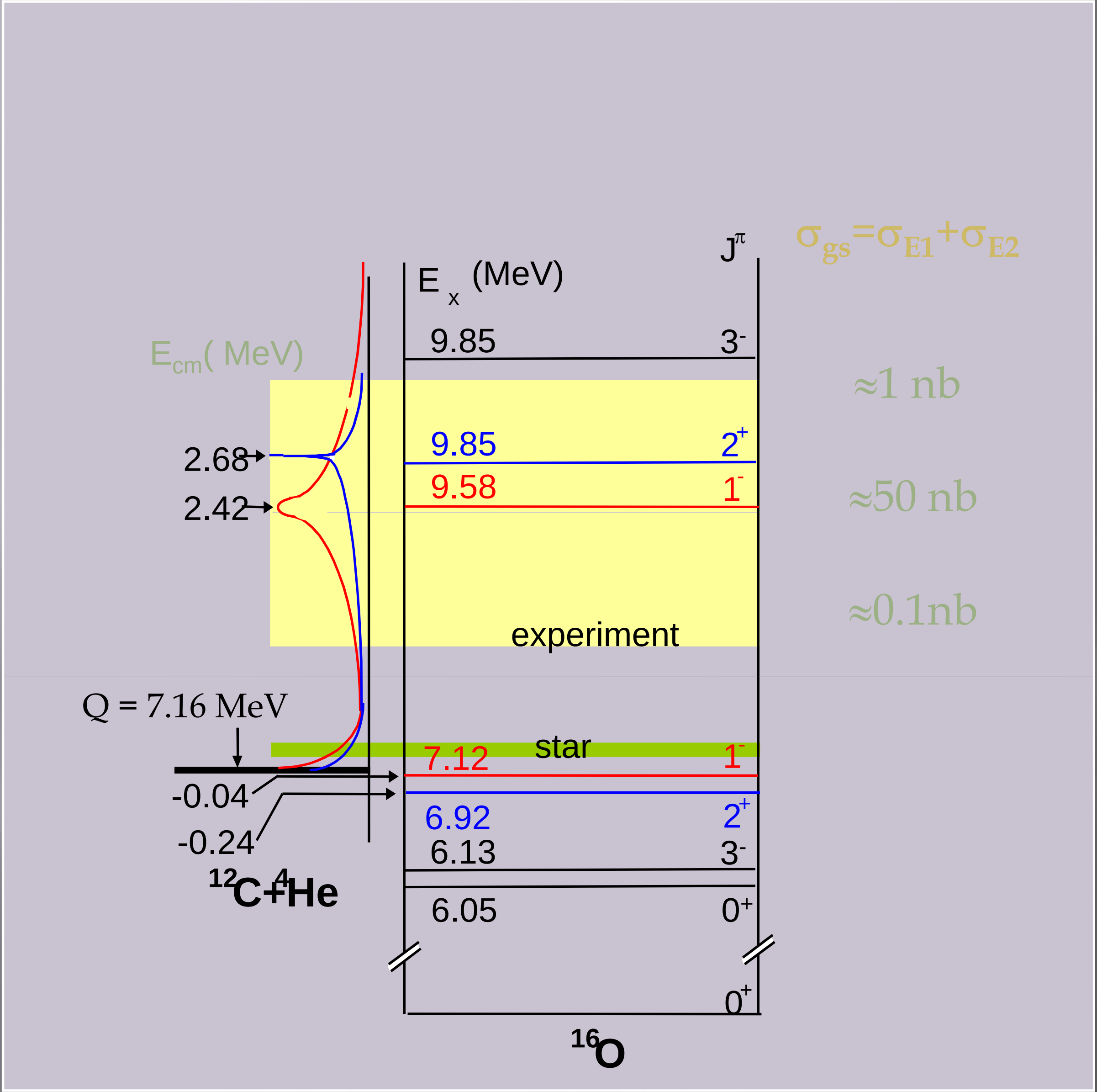
$\Phi = \Sigma_\lambda A_\lambda X_\lambda$

$\gamma_\lambda, E_\lambda$

Matching $\Phi'(r)/\Phi(r)$ at the nuclear radius

$\sigma(A_\lambda, \gamma_\lambda, E_\lambda)$

★Cross sections include contributions from few levels
★Level parameters from experimental data



Experimental data:

- $^{12}C(\alpha,\gamma)^{16}O$
- $^{12}C(\alpha,\alpha)^{12}C$
- ^{16}N β-delayed α-decay

R-matrix fit to the s_{E1}

- **Global fit**
- Least square method:
- $\chi^2=\chi^2_\beta+\chi^2_{\delta_1}+\chi^2_{\delta_3}+\chi^2_\gamma$
- **Extrapolation**
- Uncertainty on extrapolation and fitted parameters

- $^{16}N \to {}^{16}O \to {}^{12}C+\alpha$ data
- $W_\alpha(E)=F(E, a_\ell, A_{\lambda\ell}, \gamma^2_{\lambda\ell}, E_{\lambda\ell})$
- $\ell=1,3;\ \lambda=1,2,3$

- $^{12}C(\alpha,\gamma)^{16}O$
- $\sigma_{E1}(E)=H(E, a_\ell, \gamma^2_{\lambda\ell}, \Gamma^2_{\lambda\ell}, E_{\lambda\ell})$
- $\ell=1;\ \lambda=1,2,3$

- $^{12}C(\alpha,\alpha)^{12}C$
- $\delta_\ell(E)=G(E, a_\ell, \gamma^2_{\lambda\ell}, E_{\lambda\ell})$
- $\ell=1,3;\ \lambda=1,2,3$

Rmatrix code by R.E. Azuma et al., PRC 50,2(1994)1194

Least square method – uncorrelated data

- Measurement of Y in conjunction with X -> (x_i,y_i) i=1,…,n
- cov $(y_i,y_j) = E[(y_i-\langle y_i\rangle)(y_j-\langle y_j\rangle)]=V_{ij}=\delta_{ij}\cdot\sigma_{y_i}^2$, $\langle y_i\rangle = E[y_i]$
- Model $Y=f(X; A_1,\ldots,A_m)$
- $(\partial f/\partial x)\,\sigma_{x_i} \ll \sigma_{y_i}$
- $Q = \Sigma_i[y_i-f(x_i;a_1,\ldots,a_m)]^2/\sigma_{y_i}^2$

- Minimization
- hopefully: $Q \to \chi^2$ distribution with $\nu=n-m$ degree of freedom
- error matrix ε: $\mathrm{cov}(a_i,a_j)=\varepsilon_{ij}$, $\varepsilon=\alpha^{-1}$, $\alpha_{kl}=1/2\ \partial^2 Q/\partial a_k\partial a_l$

Simple example: linear case

★ Y=AX+B

I. Analytic solution (now)

II. Numeric al solution (later)

III. Graphic solution (also later)

x	y	σ_y
0	0.92	0.5
1	4.15	1.0
2	9.78	0.75
3	14.46	1.25
4	17.26	1.0
5	21.9	1.5

Example: linear case – analytic solution

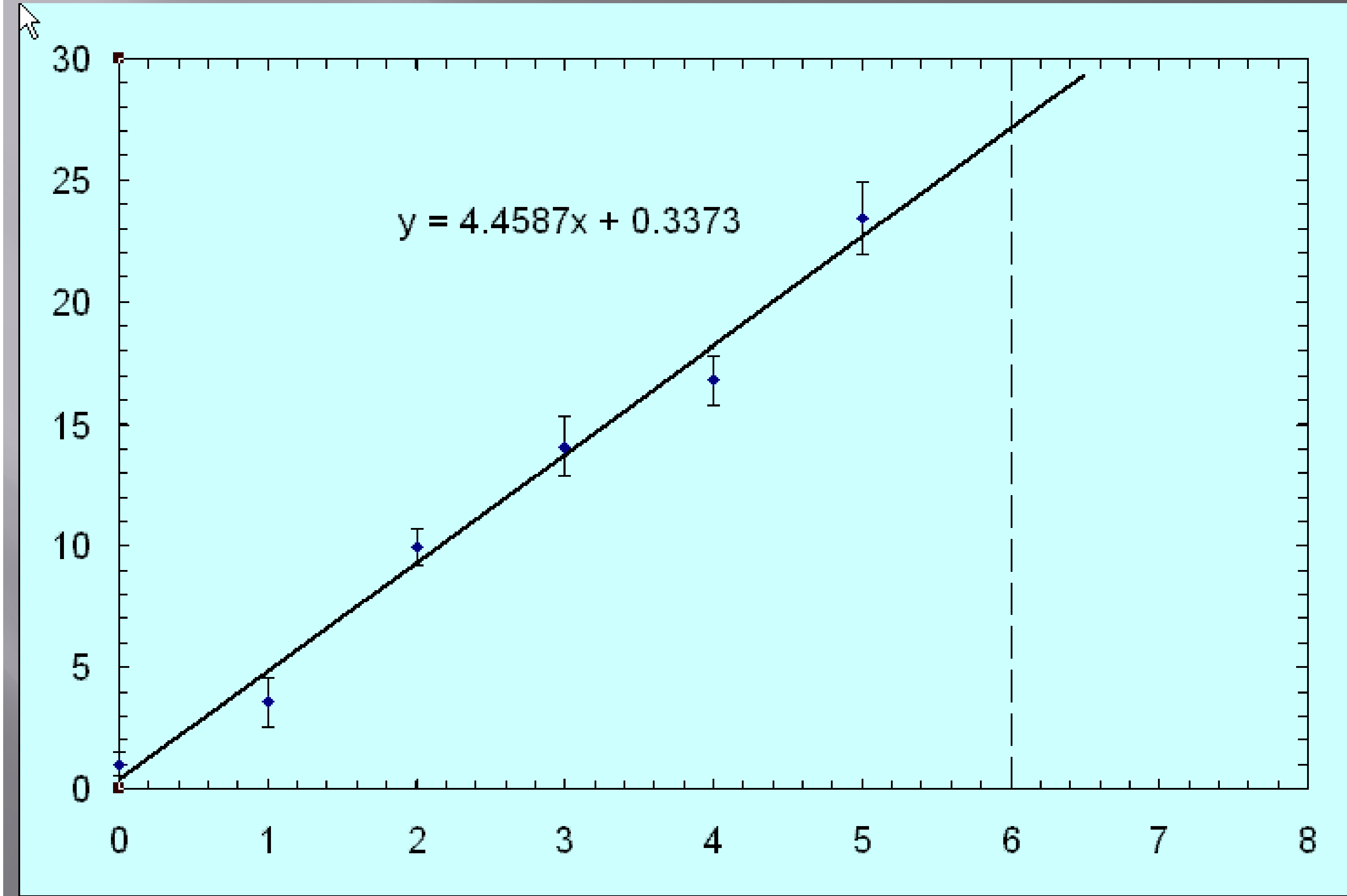
- $Q = \Sigma_i [y_i - ax_i - b]^2 / \sigma_{y_i}^2$
- $\partial Q / \partial a = -2\Sigma(y_i - ax_i - b) xi / \sigma_{y_i}^2 = 0$; $\partial Q / \partial b = -2\Sigma(y_i - ax_i - b) / \sigma_{y_i}^2 = 0$
- error matrix ε: $cov(a_i, a_j) = \varepsilon_{ij}$, $\varepsilon = \alpha^{-1}$, $\alpha = \begin{pmatrix} \partial^2 Q / \partial a^2 & \partial^2 Q / \partial a \partial b \\ \partial 2Q / \partial b \partial a & \partial^2 Q / \partial b^2 \end{pmatrix}$
- $a = 4.227$; $b = 0.879$
- $\sigma^2_a = \varepsilon_{11} = 0.044$; $\sigma^2_b = \varepsilon_{22} = 0.203$; $cov(a,b) = \varepsilon_{12} = -0.0629$
- $x^* = 6$; $y^* = y(x^*) = 26.24$
- $\sigma^2_{y^*} = (\partial y / \partial a)^2 \sigma^2_a + (\partial y / \partial b)^2 \sigma^2_b + 2\, cov(a,b)\, \partial y / \partial a\, \partial y / \partial b =$

$= x^{*2} \sigma^2_a + \sigma^2_b + 2 x^* cov(a,b) = 1.0$

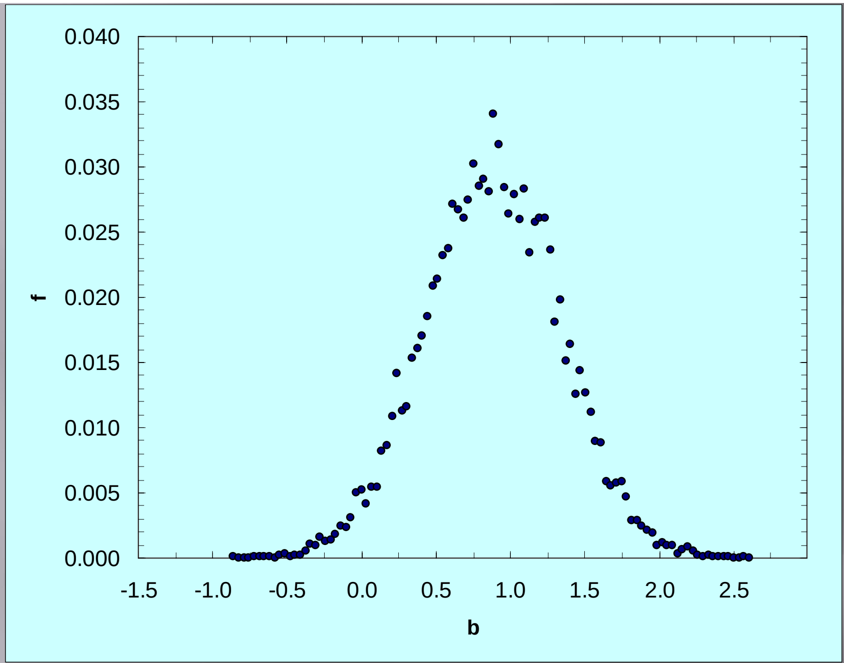
Monte Carlo estimate of the uncertainty on the extrapolation

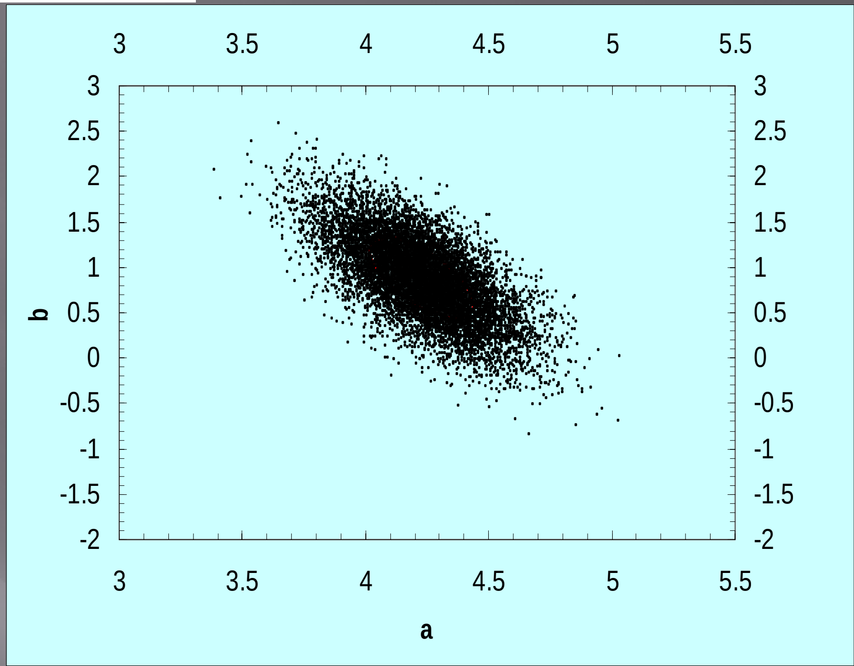
- each y_i has a normal distribution $F(< y_i >, \sigma_{y_i}^2)$
- using a (pseudo-)random number generator one can simulate a set of n possible results of repeated experiments
- For each set one estimate parameters and calculate the extrapolated value (i.e. in our example a, b, and y*)
- The analysis of the distributions obtained provides the best estimate of and the corresponding variances a, b, y*,

Gialanella et al Eur. Phys. J. A 11 (2001)

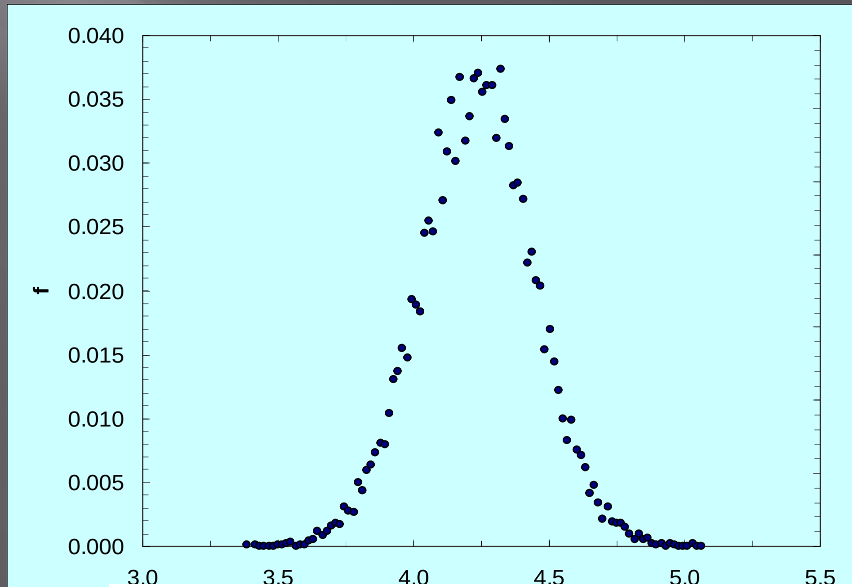

y = 4.4587x + 0.3373
30
25
20
15
10
5
0
0
1
2
3
4
5
6
7
8

Example: linear case – Monte Carlo

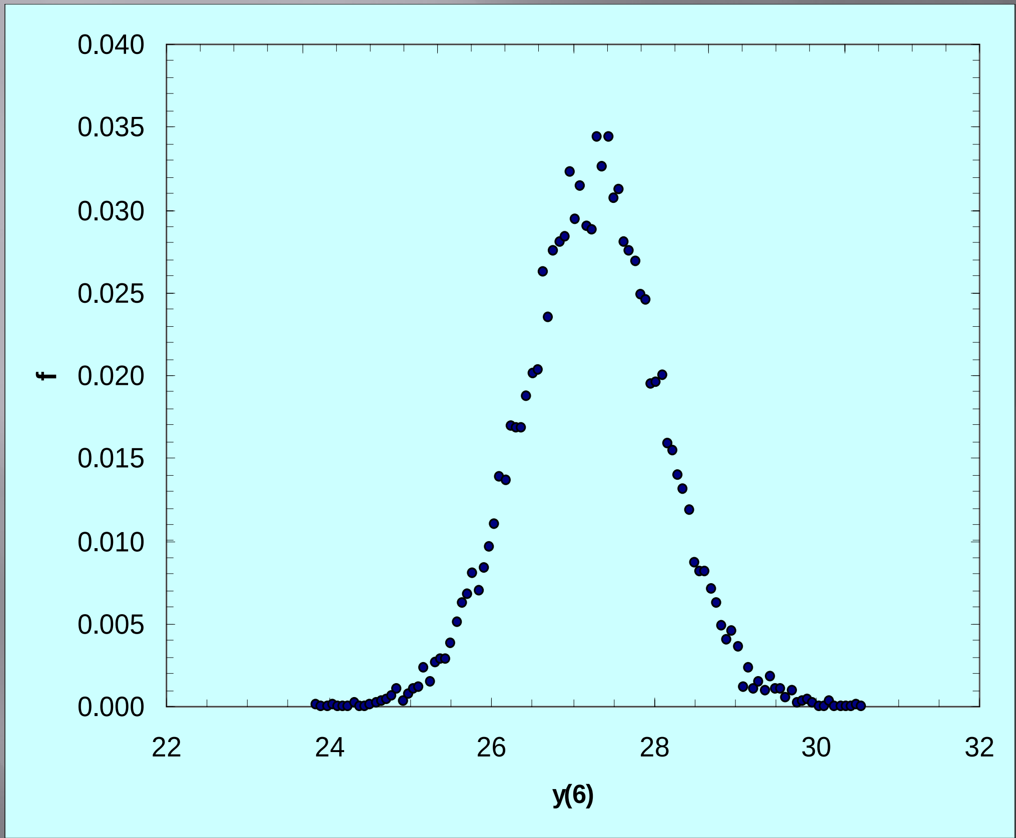




- ★N=10000
- ★a=4.231 ; b=0.873
- ★ σ^2_a= 0.044 ; σ^2_b = 0.200; cov(a,b)=-0.0631
- ★ analytical: a=4.227 ; b=0.879
- ★ σ^2_a= 0.044 ; σ^2_b = 0.203; cov(a,b)=-0.0629



Example: linear case – Monte Carlo



- ★ $x^*= 6$; $y^*= y(x^*)=26.26$
- ★ $\sigma^2_{y^*}=1.02$
- ★ analytical: $\underline{y^*}= \underline{26.24}$;
- ★ $\sigma^2_{y^*}=1.0$

Another method

- In the linear case, 1 parameter
- Taylor expansion around the minimum:

$\chi^2=\chi^2_{min}+ 1/2\ \partial^2\chi^2/\ \partial a^2\ \ (a-a_{min})^2$

- but $\sigma_a{}^2=|1/2\ \partial^2\chi^2/\ \partial a^2|^{-1}$ -> if $a=a_{low}=a_{min}-\sigma_a$ or $a=a_{high}=a_{min}+\sigma_a$

  then $\chi^2=\chi^2_{min}+ 1$

- Many parameters: pay attention to correlation
- Non linear case: pay attention to strong asymmetry

  i.e. $(a_{min}-a_{low})\neq(a_{high}-a_{min})$

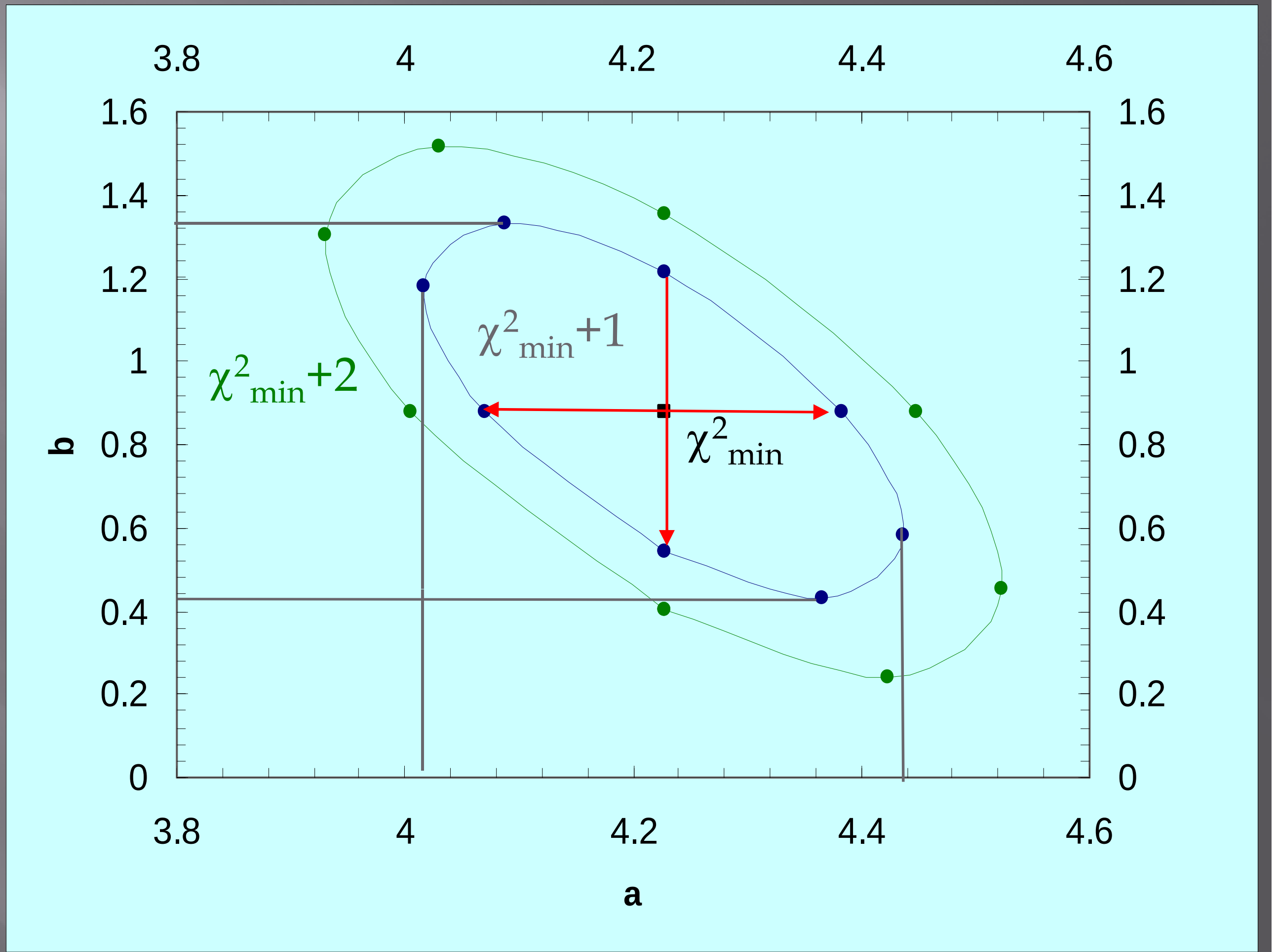
★ a=4.227 ; b=0.879

★ σ^2_a= 0.044 ; σ^2_b = 0.203

★ error matrix for cov(a,b)

★ σ^2_a= 0.024 ; σ^2_b = 0.113

i.e. don't forget covariance



What's about normalization errors?

In some cases they are neglected in the fit, and later used to estimate the uncertainties. A bettar procedure is to fit the unnormalized(i.e. uncorrelated data):

- ★ let $y_{i_k,k}=c_k\, z_{i_k,k}$ k=1,..,n be n measurements with i_k=1,..,n_k points each
- ★ Model $Y_k=f_k\,(X_k;\, A_1,\ldots,A_m)$
- ★ $Q = \Sigma_k \{\Sigma_{i_k} [z_{i_k,k} - f(x_i;a_1,\ldots,a_m)/c_k]^2/\sigma_{y_{ik}}{}^2 + (c_k - a_{m+1})^2/\sigma_{c_k}{}^2]\}$
- ★ hopefully: Q->χ^2 distribution with $\nu = \Sigma_k\, n_k$ -m – n degrees of freedom

G. D'Agostini, NIM A 346(1994)306 and references tl

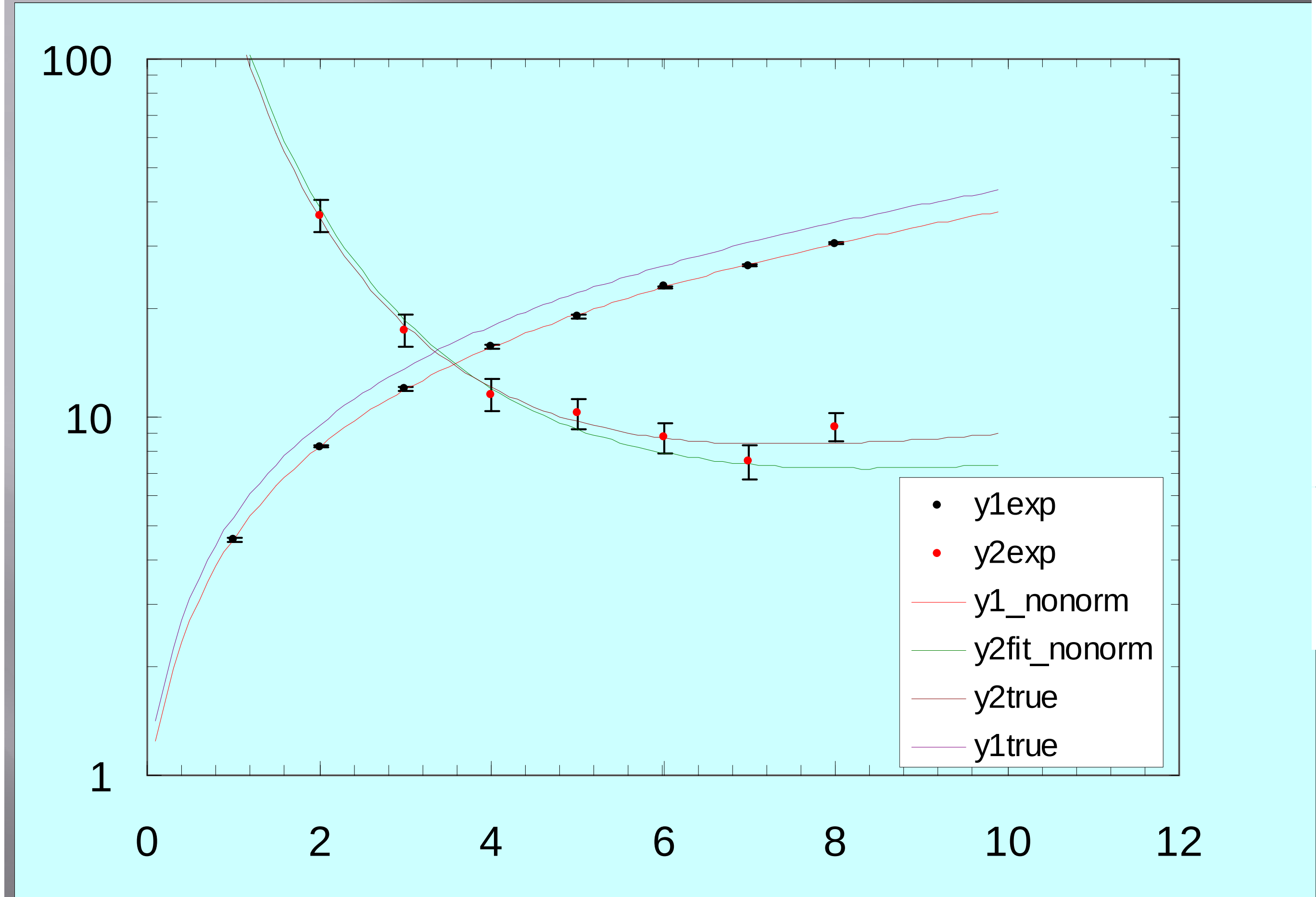
An example

- $Y_1=f_1(X;A_1,A_2,A_3)=A_1+\mathrm{sqrt}(A_2)\cdot X$
- $Y_2=f_2(X;A_1,A_2,A_3)=A_1+A_2\cdot X/3+A_3^{-2}\cdot X^3$

- Experiment:
- $\sigma_{y_{1i}}/y_{1i}=0.01$
- $\sigma_{c_1}/c_1=0.1$
- $\sigma_{y_{1i}}/y_{1i}=0.1$
- $\sigma_{c_2}/c_2=0.01$

- True parameter values
- $A_1=1$; $A_2=2$; $A_3=3$;
- Normalization:
- $y_1=c_1\cdot y_1$
- $y_2=c_2\cdot y_2$
- True normalization values
- $c_1=1.2$; $c_2=1$

Fit without normalization constants

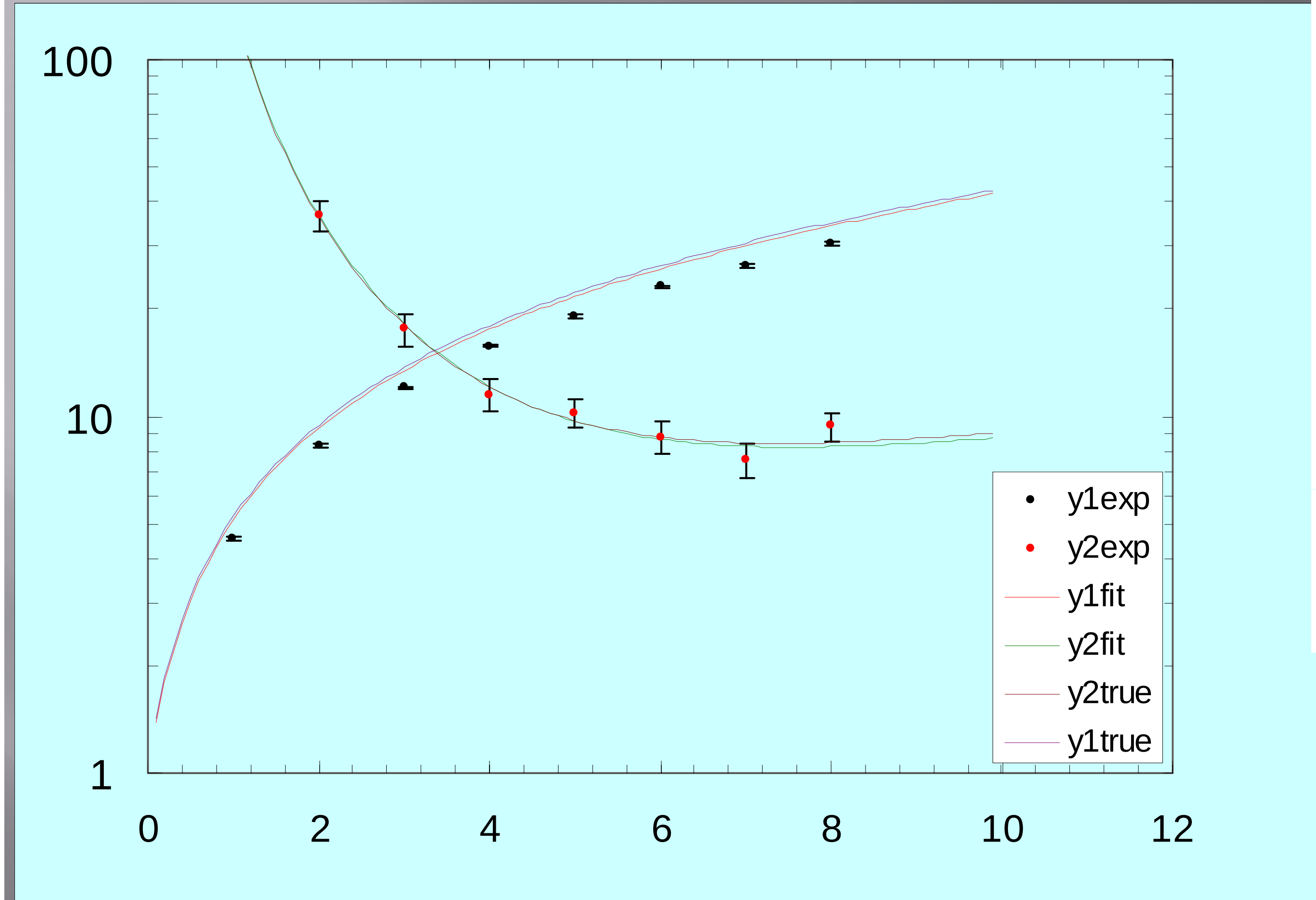


★ fit:
★ A_1=0.87 (exp.1)
★ A_2=1.52 (exp.2)
★ A_3=3.08 (exp.3)

★ $\chi^2=14.4$
★ $\nu=13$
★ $\chi^2/\nu=1.11$

★ experimental :
★ $c_1=1.04\pm0.12$ (1.2)
★ $c_2=0.99\pm0.01$ (1)

Fit with normalization constants

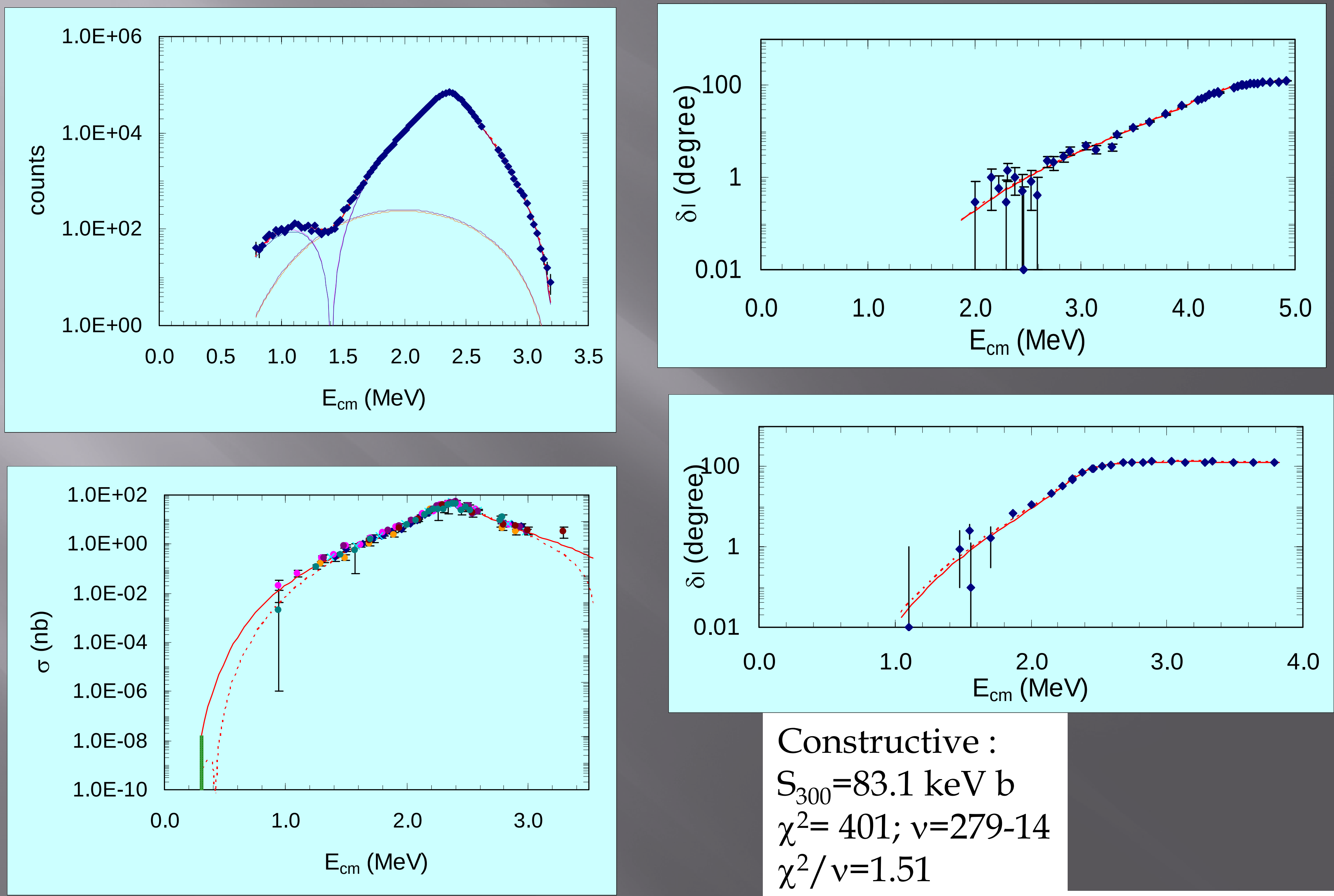


- ★ fit:
- ★ A_1=0.97 (exp.1)
- ★ A_2=1.91 (exp.2)
- ★ A_3=3.02 (exp.3)

- ★ χ^2=9.2
- ★ ν=11
- ★ χ^2/ν=0.84

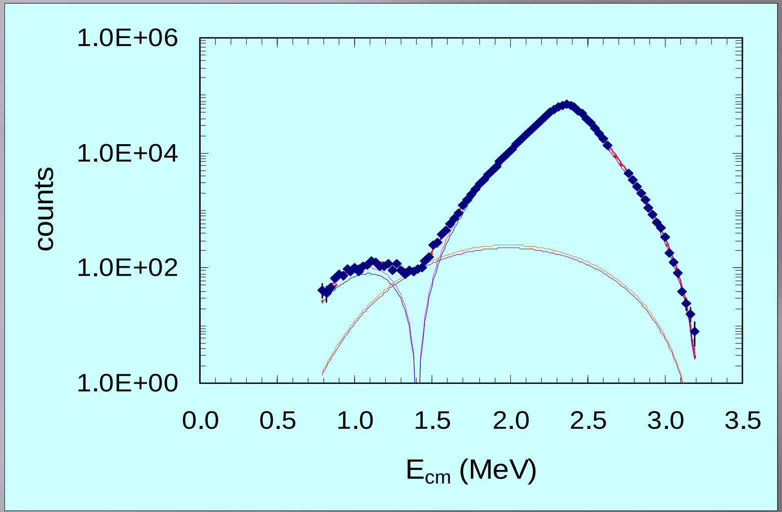
- ★ c_1=1.17 (exp 1.2)
- ★ c_2=0.99 (exp 1)

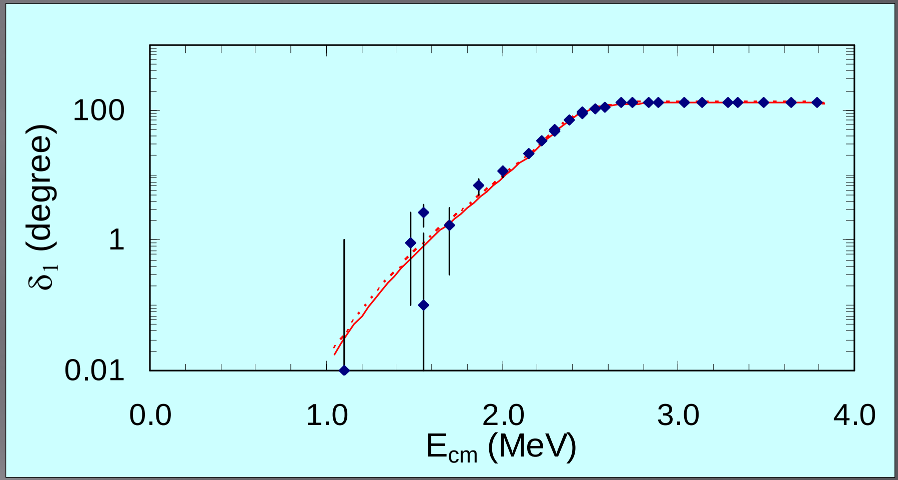
R-matrix fit to the s_{E1} - no normalization

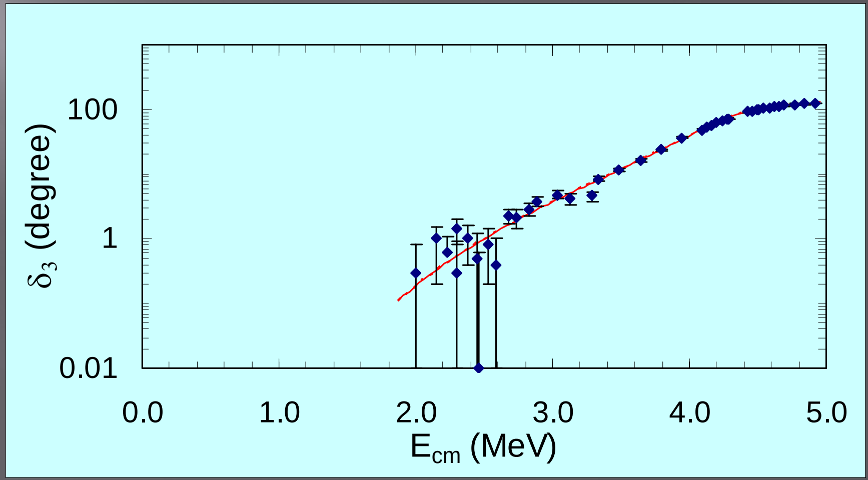


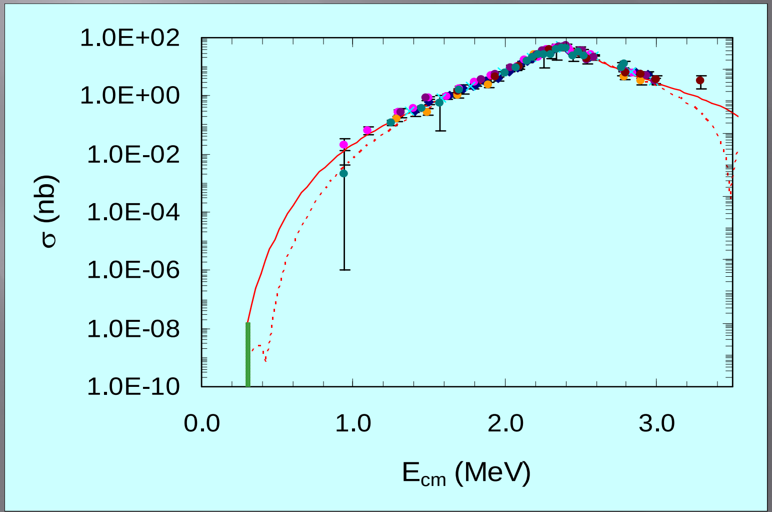
Constructive :
S_{300}=83.1 keV b
χ^2= 401; ν=279-14
χ^2/ν=1.51

R-matrix fit to the s_{E1} - with normalization





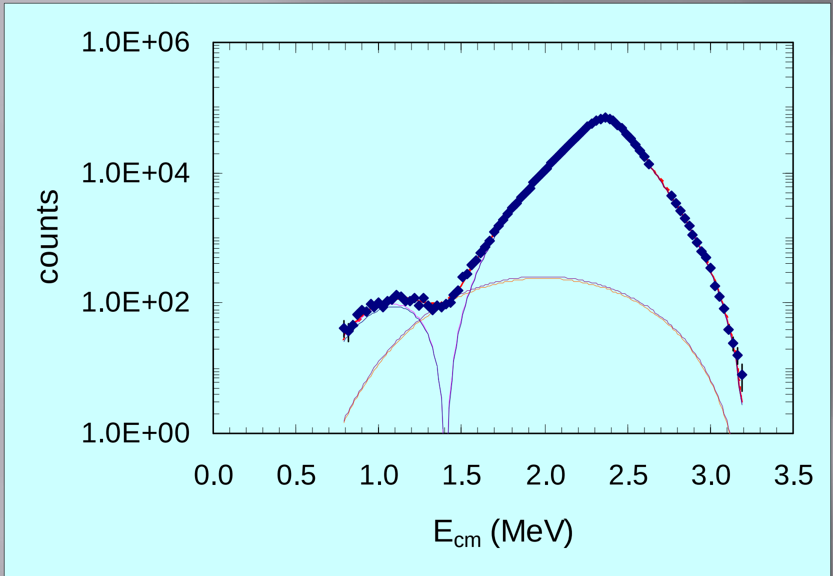


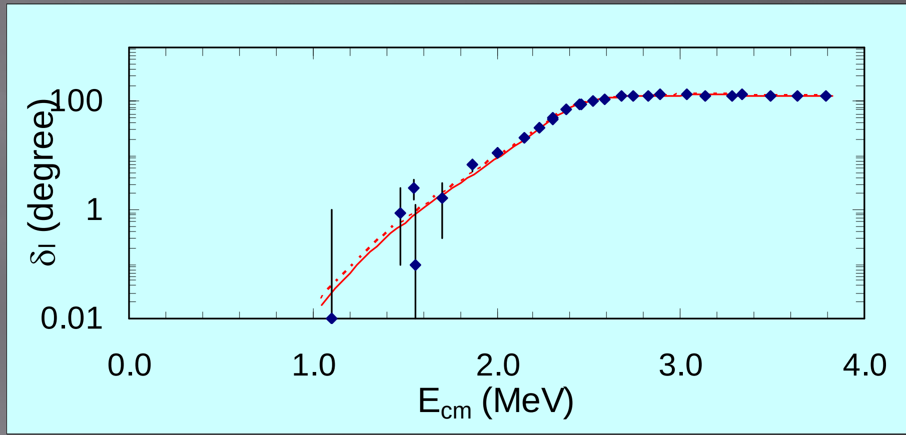


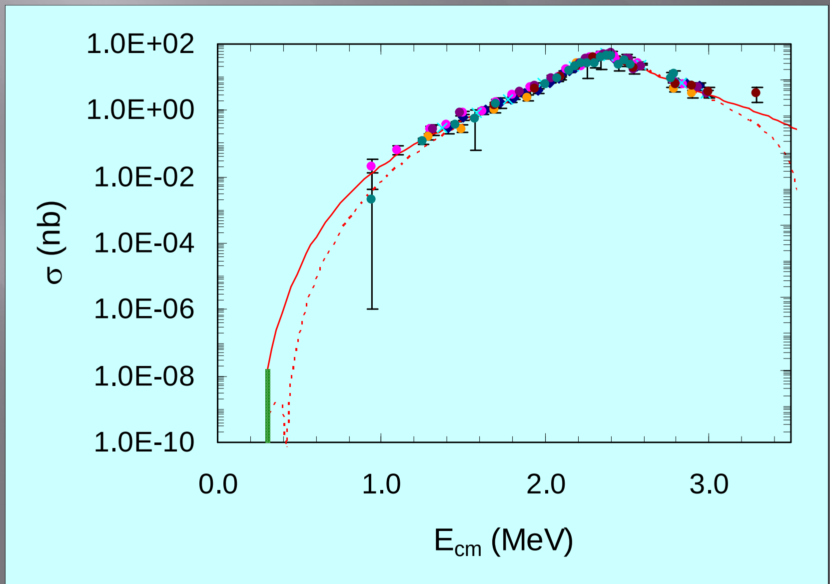
Constructive :
S_{300}=86.4 keV b
χ^2= 352; ν=279-14
χ^2/ν=1.38

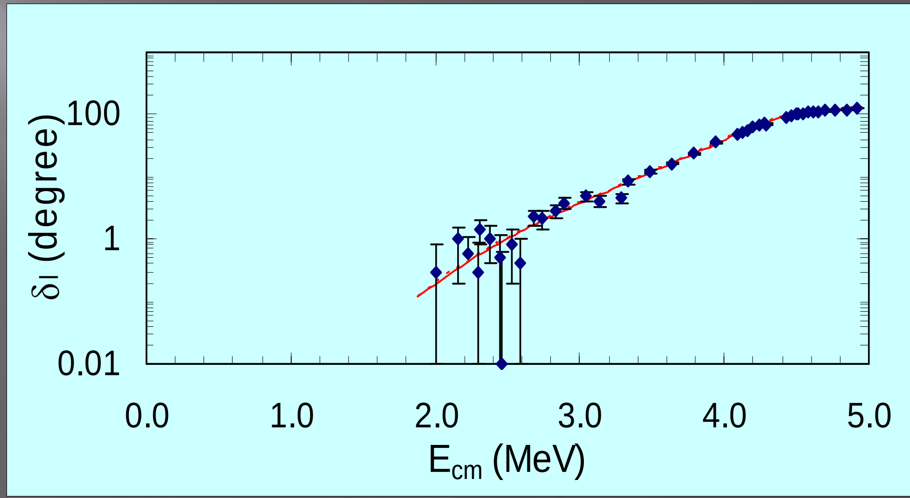
L. Gialanella- SLENA 2012, Kolkata, India

R-matrix fit to the s_{E1} - no normalization









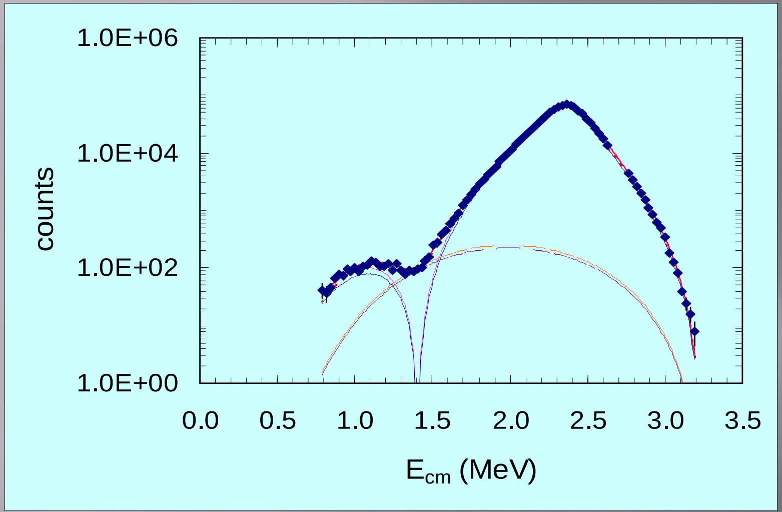
Destructive :

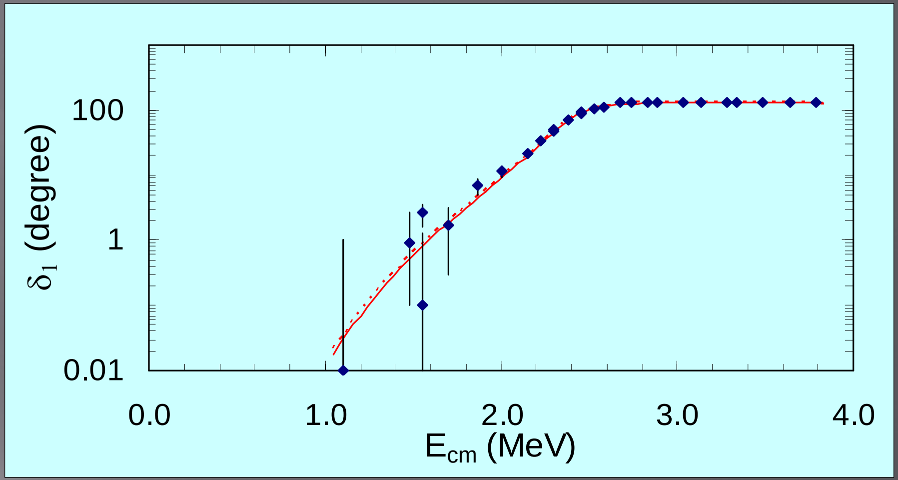
S_{300}=2.5 keV b

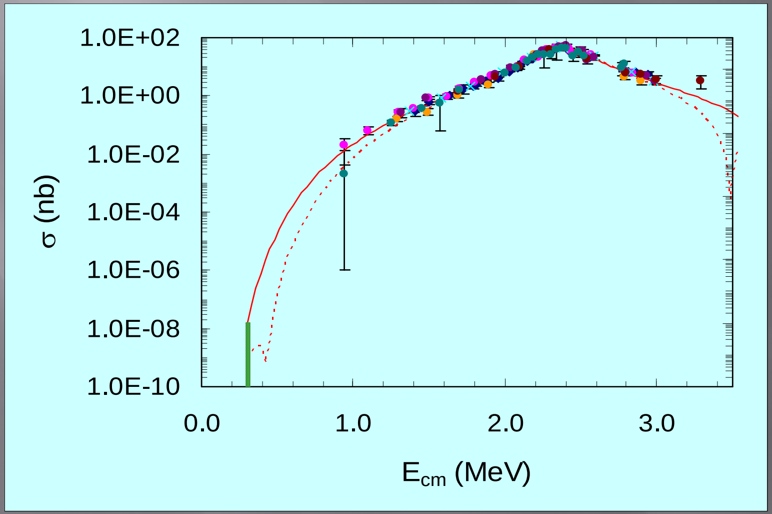
χ^2= 547; ν=279-14

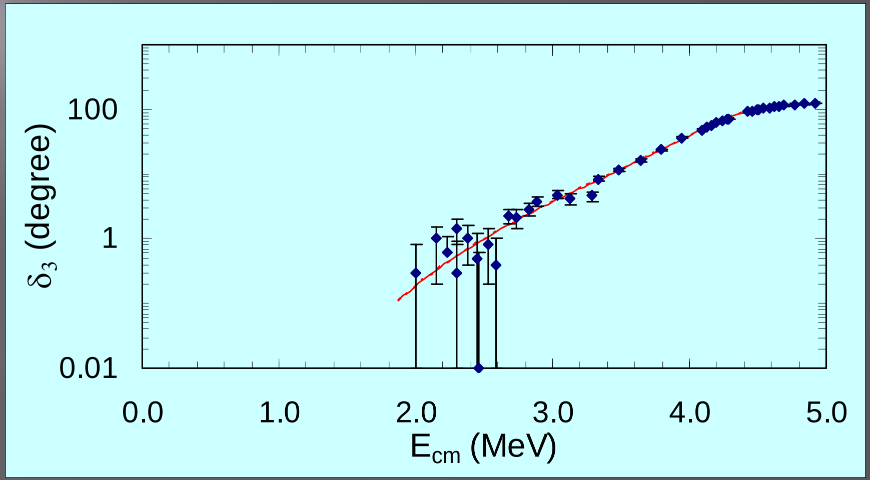
χ^2/ν=2.06

R-matrix fit to the s_{E1} – with normalization



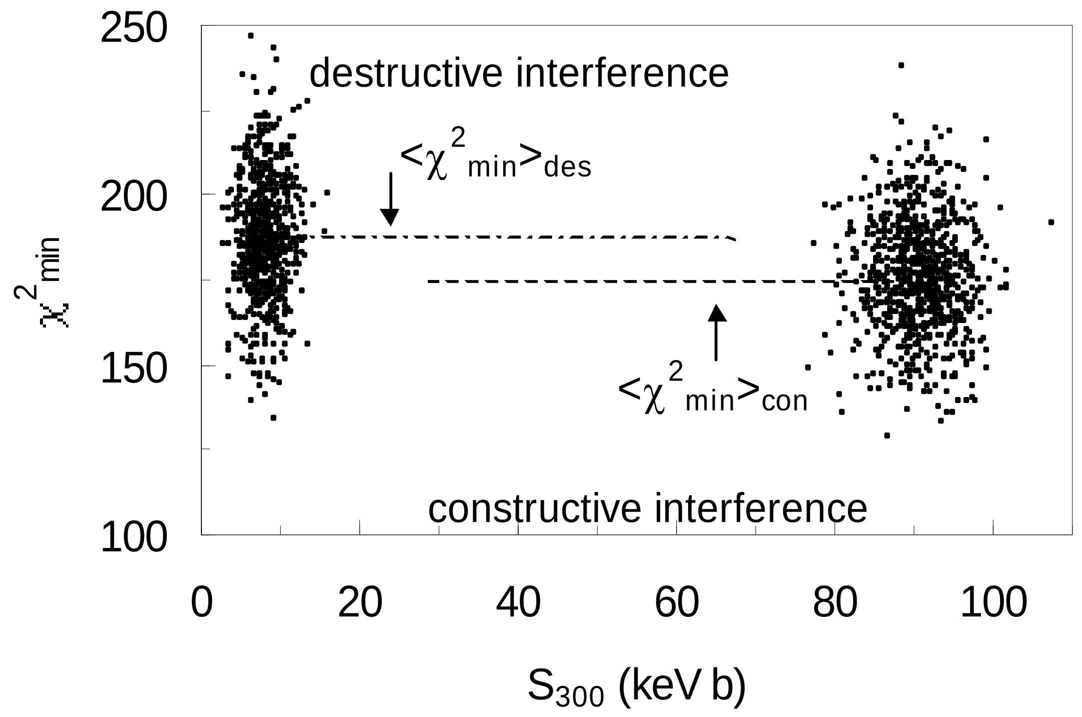


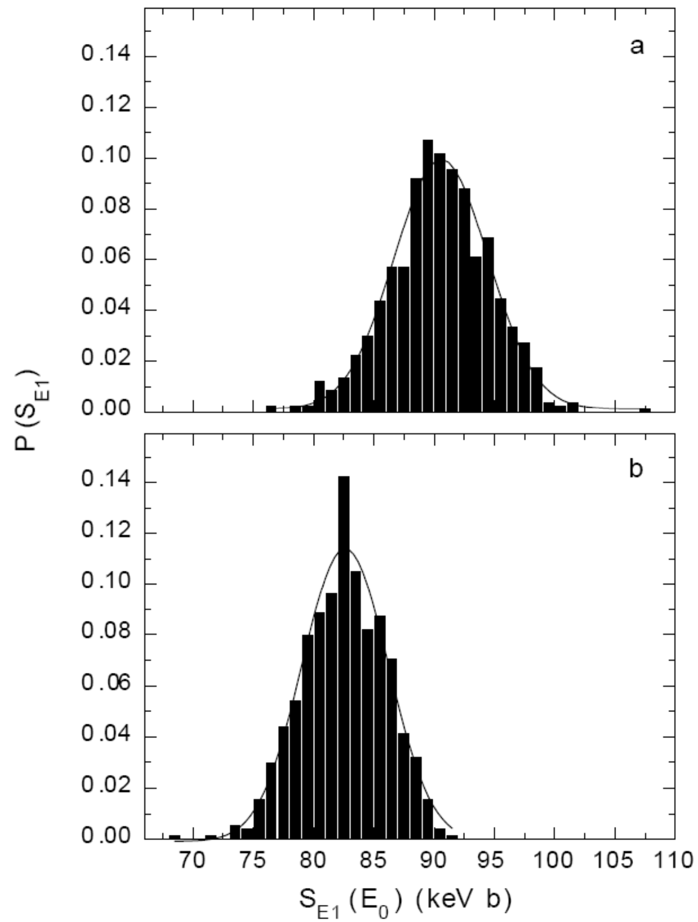




Destructive :
S_{300}=3 keV b
χ^2= 500; ν=279-14
χ^2/ν=1.96

Rmatrix - Monte Carlo





For a full calculation, including normalization and using MonteCarlo, see D. Schürmann et al., PLB 2012

summary

- To which cases do these consideration apply?
  - Efficiency
  - calibration
  - Relative measurements
  - etc
- So: to which cases these consideration do not apply?
  - few
- Special attention must be paid to high precision experiments