UNIVERSITAT POLITÈCNICA DE CATALUNYA

MANTID

ISIS

FABADA implementation into Mantid

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Contents

- Bayesian vs. Frequentist Analysis
- FABADA algorithm
- Model selection
  - Example with synthetic data
- How to use FABADA with Mantid
  - Example with ISIS data

Frequentist analysis

Assumptions

- There only exists one χ^2 minimum (global and local)
- χ^2 has Quadratic dependence on each parameter
- Errors calculations usually disregard correlations

Results

- $P \pm \delta P$
- χ^2 minimum
- Limited model selection

Bayesian analysis

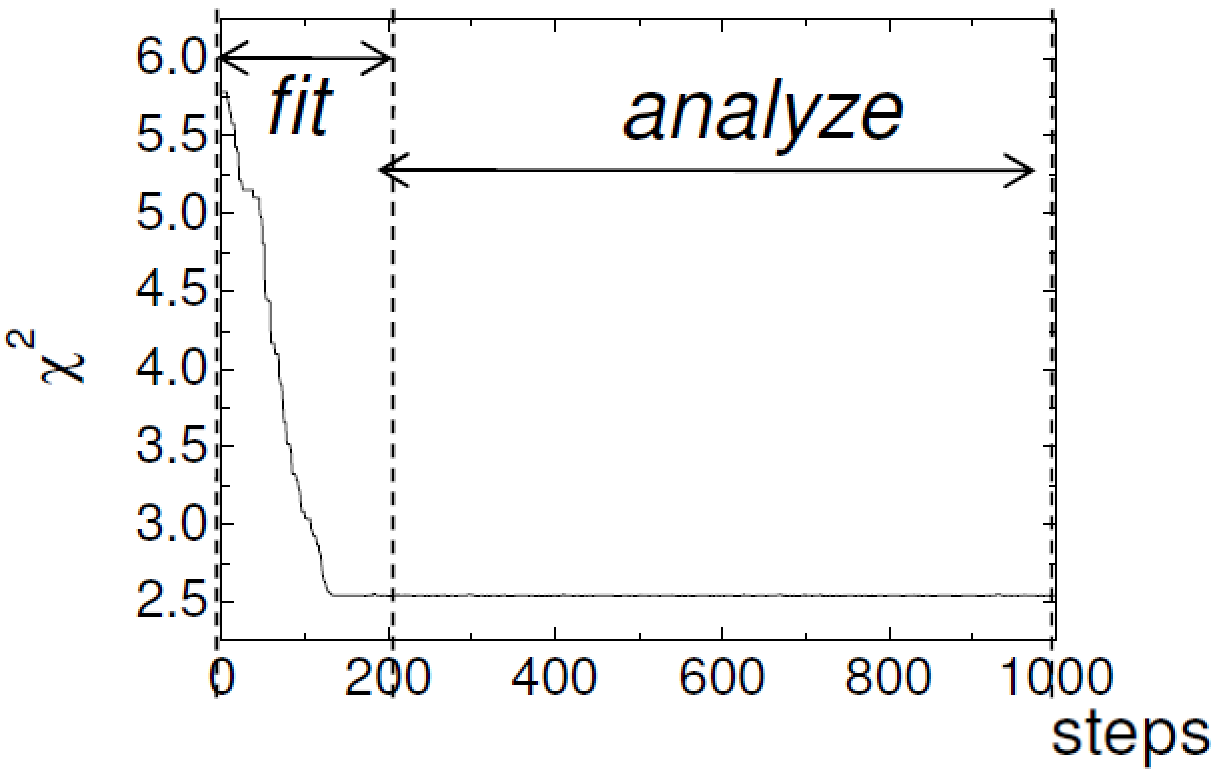
Why?

- Do not involve any assumption
- Do not get stuck in local minima of χ^2 hypersurface (for complex models)
- Improves parameter estimation
- Gets parameters correlation explicity
- Improves model selection

How?

- Let’s see…

Fitting in the χ^2 landscape



Cost function:

$$\chi^2 = \sum_{k=1}^{n} \frac{(H_k\{P_i\} - D_k)^2}{\sigma_k^2}$$

From Bayes Theorem:

$$P(D_k \,|\, H_k) \propto \exp\left(-\frac{\chi 2}{2}\right)$$

Markov Chain Monte Carlo (MCMC)

Parameter generation $$P_i^{\mathrm{new}} = P_i^{\mathrm{old}} + (\mathrm{RND} - 0.5) \cdot 2\Delta P_i^{\max}$$

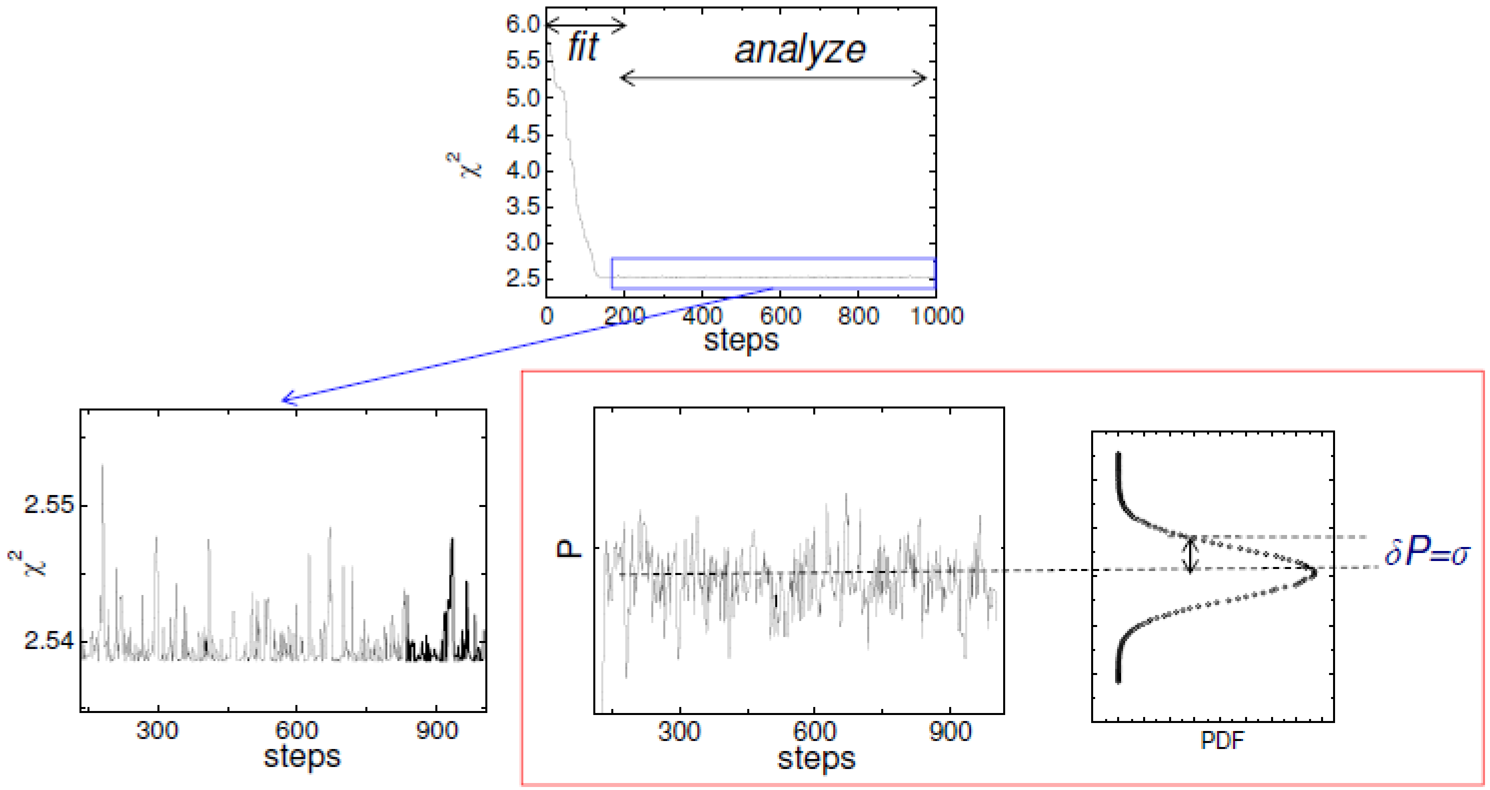
Parameter acceptance

$$\begin{cases} \chi^2_{new} < \chi^2_{old} & \text{New parameter value accepted} \\ \chi^2_{new} > \chi^2_{old} & \dfrac{P(H(P_i^{\mathrm{new}})\,|\,D_k)}{P(H(P_i^{\mathrm{old}})\,|\,D_k)} = \exp\left(-\dfrac{\chi^2_{\mathrm{new}} - \chi^2_{\mathrm{old}}}{2}\right) \end{cases}$$

Adjusting step size $\Delta P_i^{\max}$: $$\Delta P_i^{max,new} = \Delta P_i^{max,old} \cdot \frac{R_i}{R_{i,desired}}$$

where Ri = acceptance rate

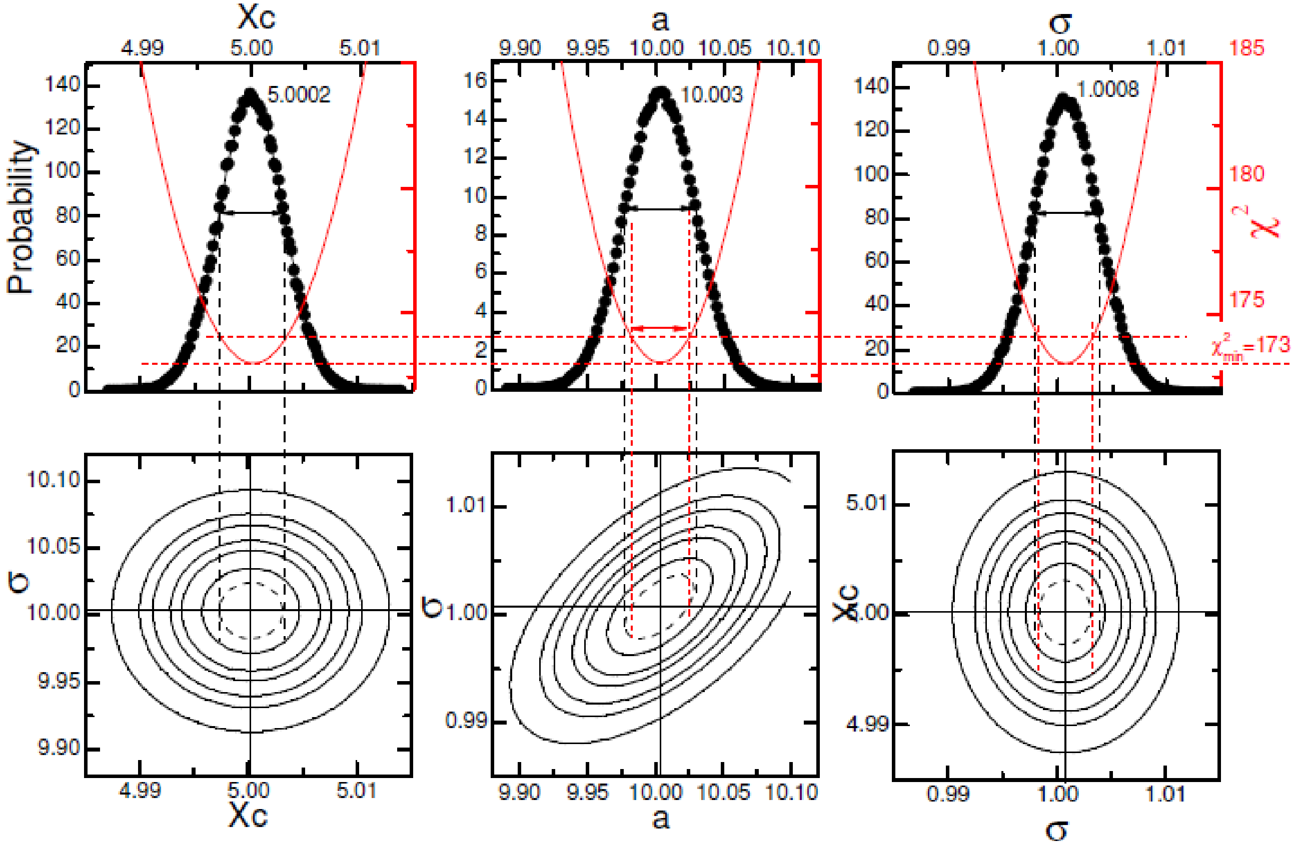
Parameter estimation



Parameter estimation:
Parameters are obtained as PDF's not as P±δP

Parameter correlations

Correlation between parameters are automatically had into account

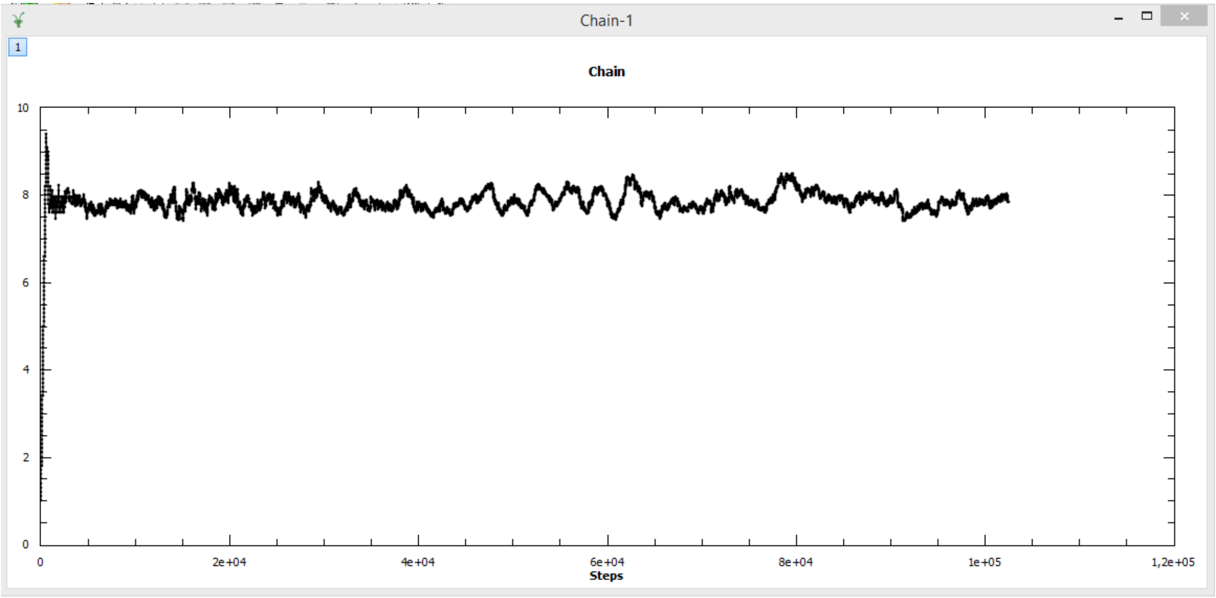


FABADA features

- Chain length
- Saving Rate
- Convergence Criteria (1%)

$$\frac{\chi^2_{old} - \chi^2_{new}}{\chi^2_{old}}$$

- Acceptance Rate = 2/3

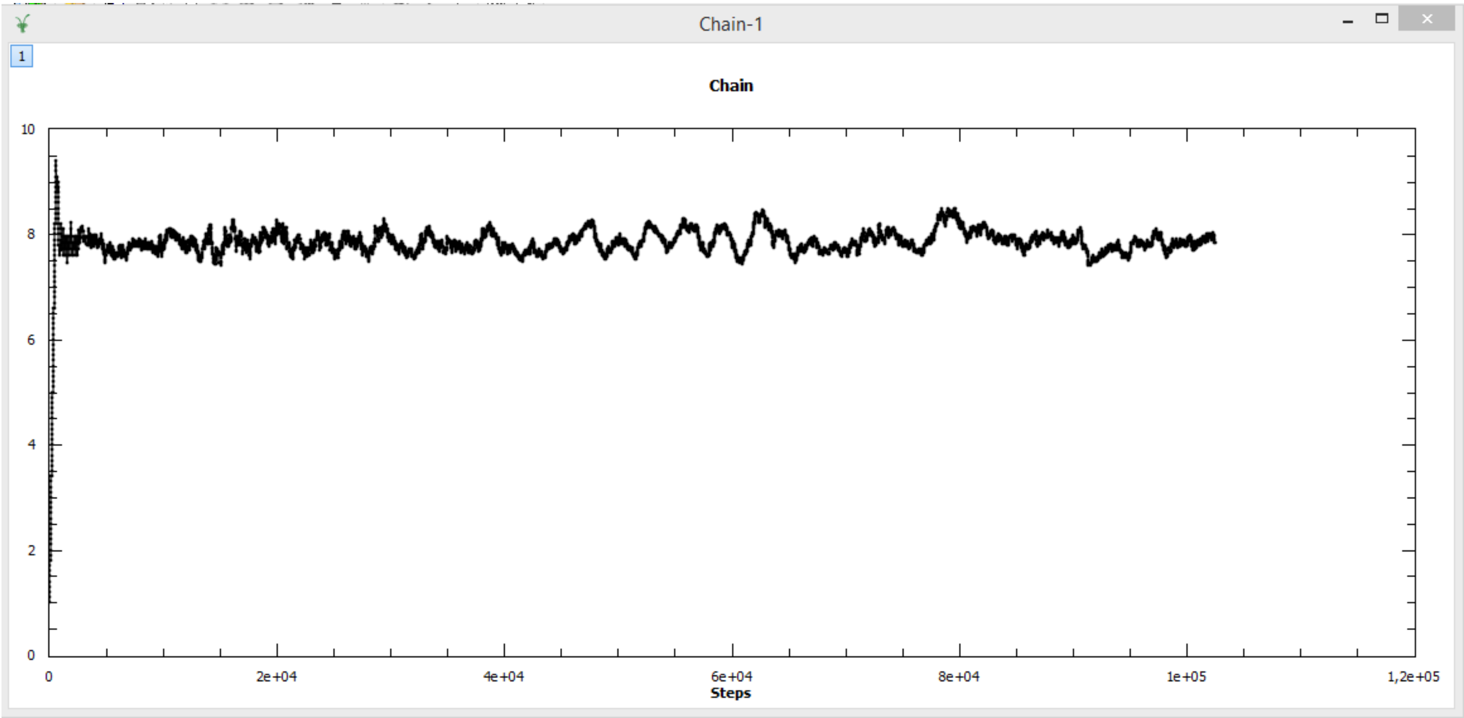


Resulting workspaces in Mantid

- Chains
- Converged Chains
- Probability density Functions (PDF)
- Cost Function Values
- Parameters values and errors

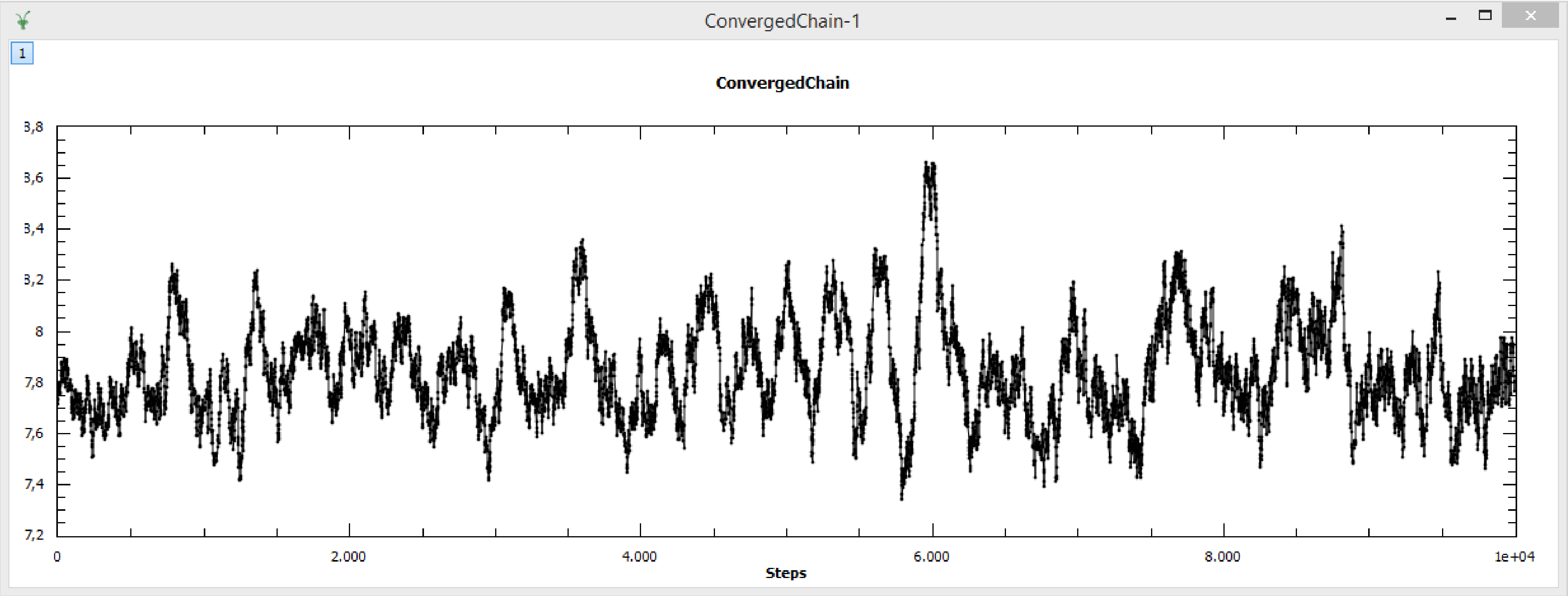
Resulting workspaces in Mantid

- Chains



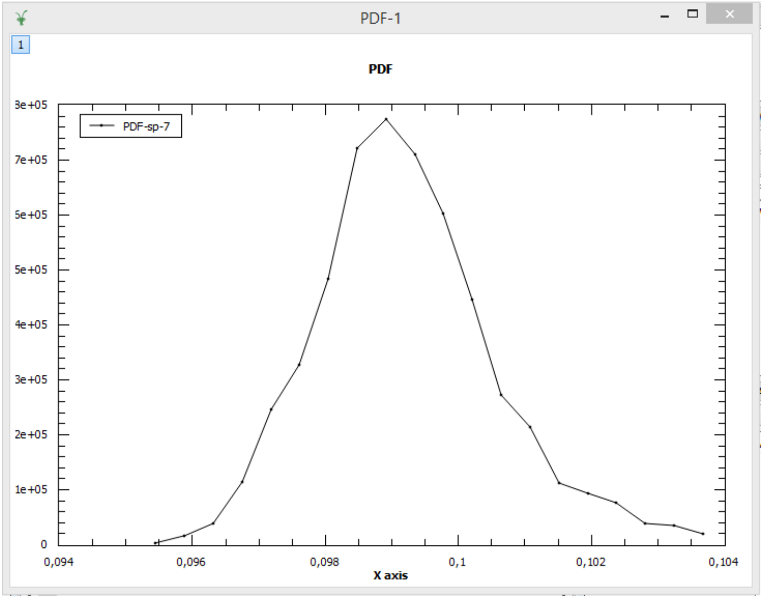
Resulting workspaces in Mantid

- Converged chains

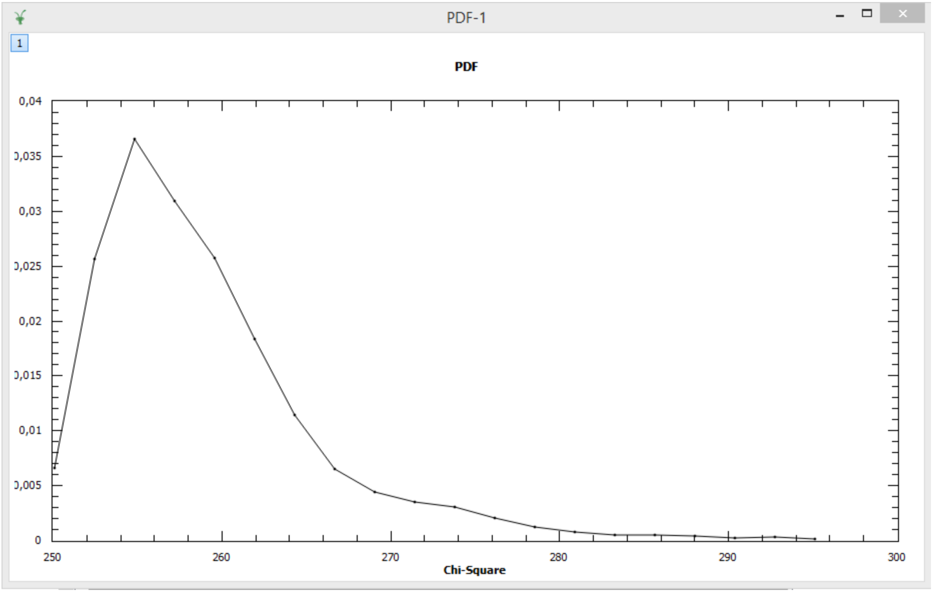


Resulting workspaces in Mantid

- Probability density Functions (PDF)



Parameter PDF



χ^2 PDF

Resulting workspaces in Mantid

- Cost Function Values

Table-2 - CostFunction

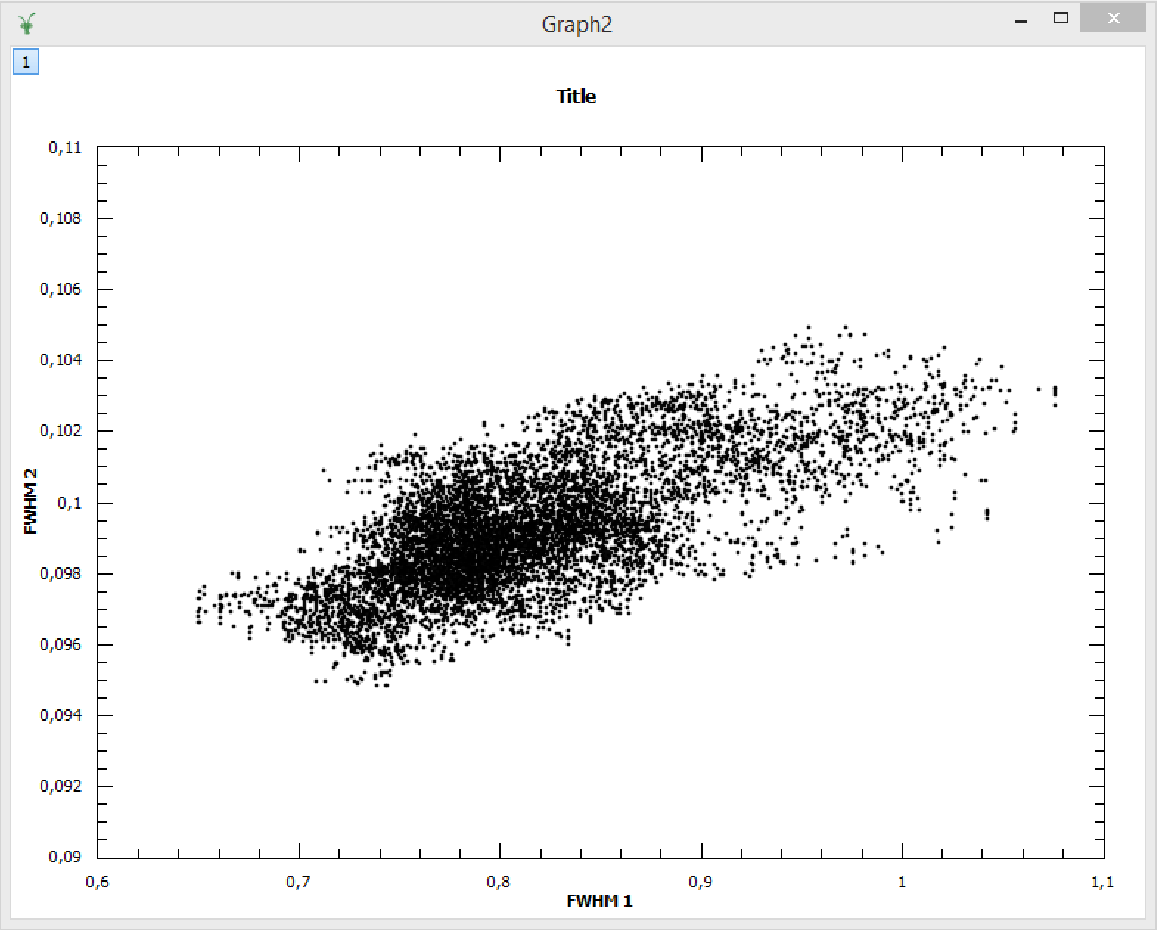
	Chi2min[Y]	Chi2MP[Y]	Chi2min_red[Y]	Chi2MP_red[Y]
0	248.611	254.741	0.504282	0.516716

- Parameters values and errors

Table-3 - Parameters

	Name[Y]	Value[Y]	Left's error[Y]	Rigth's error[
0	f1.f0.Height	7.54702	-0.062035	0.207449
1	f1.f1.Amplitude	7.79496	-0.174304	0.189859
2	f1.f1.PeakCentre	-0.00704959	-0.0153785	0.00560339
3	f1.f1.FWHM	0.787343	-0.0588715	0.0713501
4	f1.f2.Amplitude	12.6584	-0.295887	0.21955
5	f1.f2.PeakCentre	-0.00166985	-0.000783102	0.00049764
6	f1.f2.FWHM	0.0990264	-0.00121856	0.00125753

Correlations with FABADA



Model selection

Usual methods:

- “Guide to the eye” method
- Minimum χ^2 value
- The reduced χ^2 method:

$$\chi^2_{red} = \frac{\chi^2}{n-m}$$

n = number of points
m= number of parameters

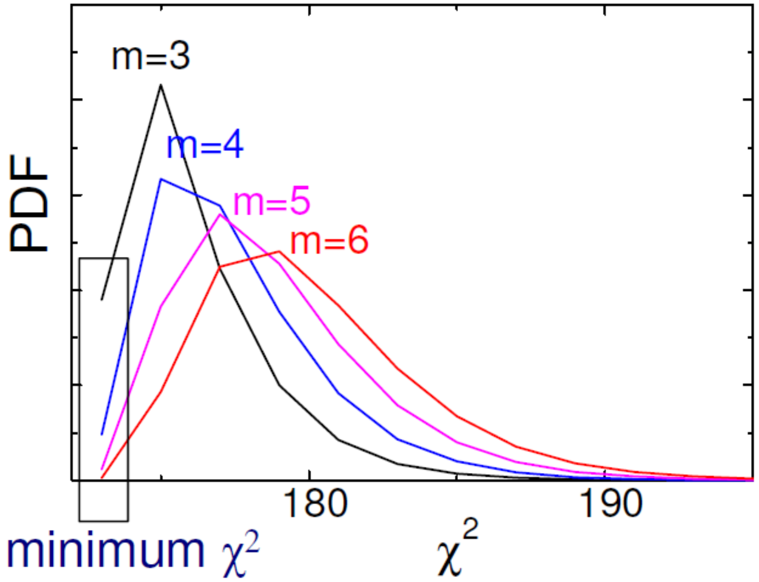
This only Works if:

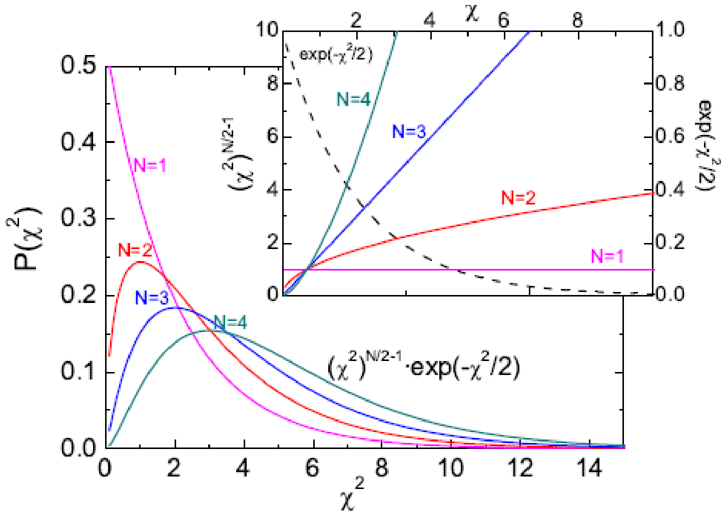
- ✓ There is no correlation between parameters
- ✓ The PDF in all parameters is Gaussian
- ✓ The minimum is not multimodal

Bayesian method

Directly compares the PDF related to χ^2

$$P(\chi^2) \propto (\chi^2)^{\frac{N}{2}-1} \cdot e^{\frac{-\chi^2}{2}}$$

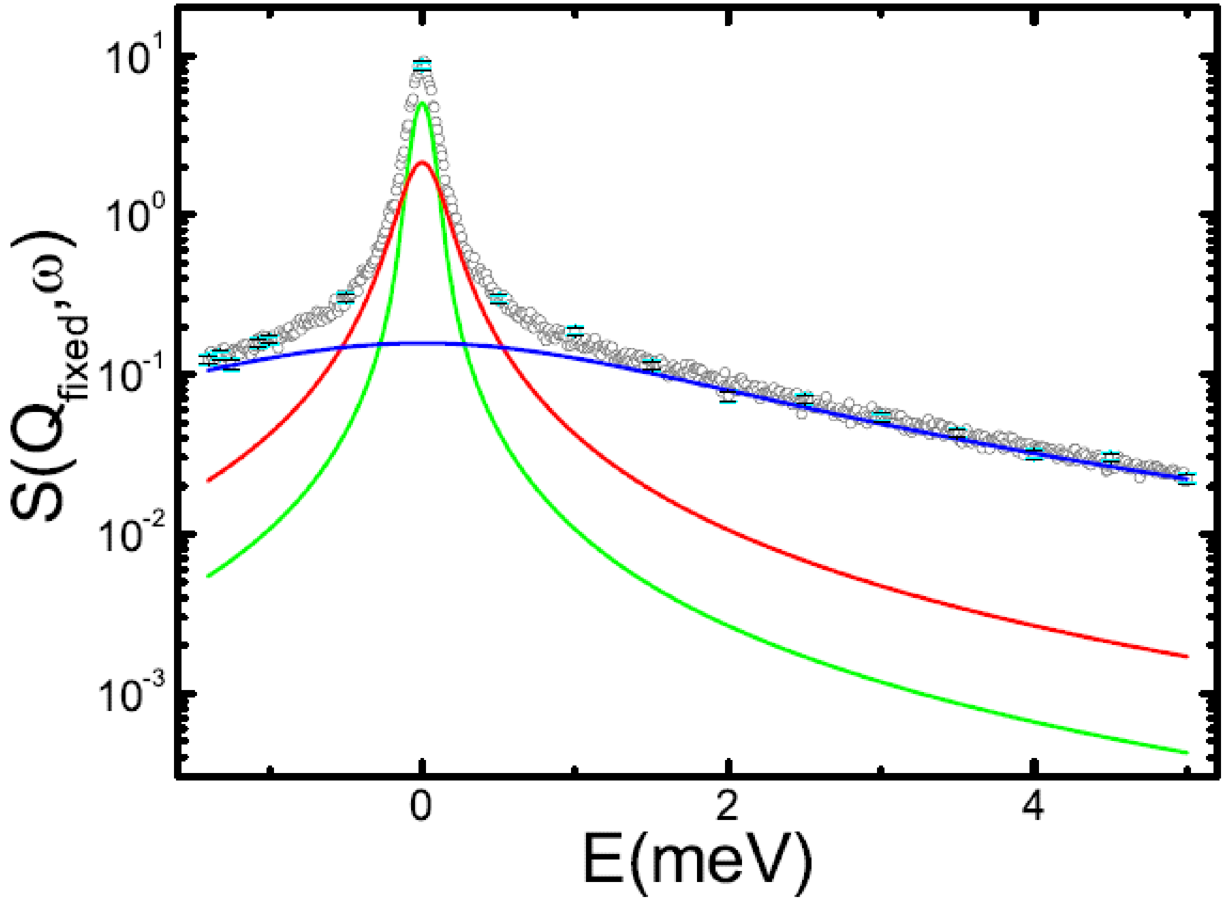




Ref. Sivia D.S. Data Analysis

An increasing number of parameters broadens the χ^2 PDF

How many lines are there?



How many lines are there?

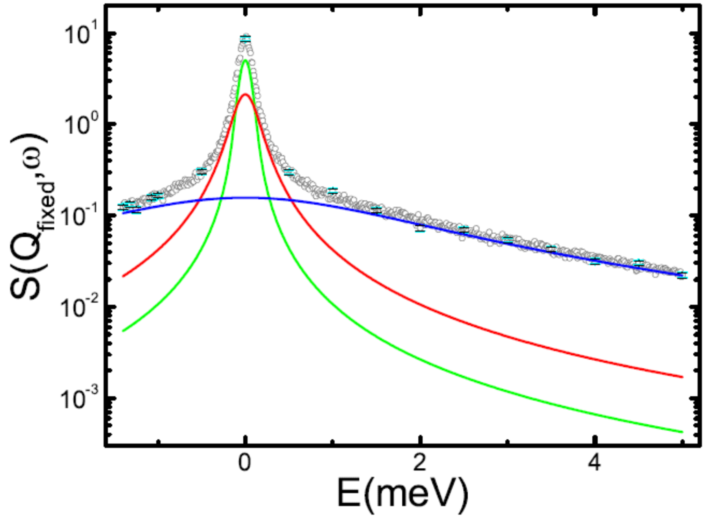
$$R \otimes (L_1 + L_2 + L_3)$$

$$L = \frac{A}{\pi}\left(\frac{\frac{FWHM}{2}}{(x-x_0)^2 + \left(\frac{FWHM}{2}\right)^2}\right)$$

$$R = e^{\left(-\frac{4\ln(2)\cdot x^2}{0.01}\right)}$$

Gaussian-distributed relative error of 6% added after convolution

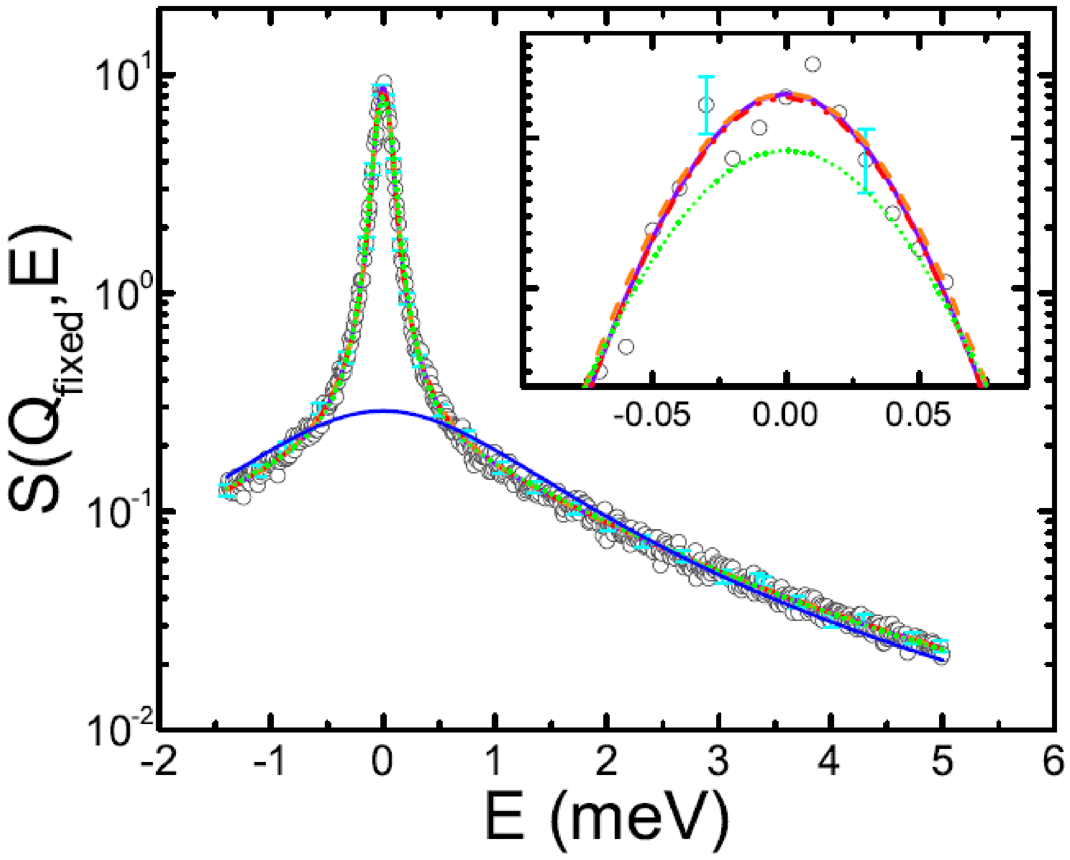
Peak	A	FWHM	x_0
L_1	1	0.04	0
L_2	1	0.4	0
L_3	1	2	0



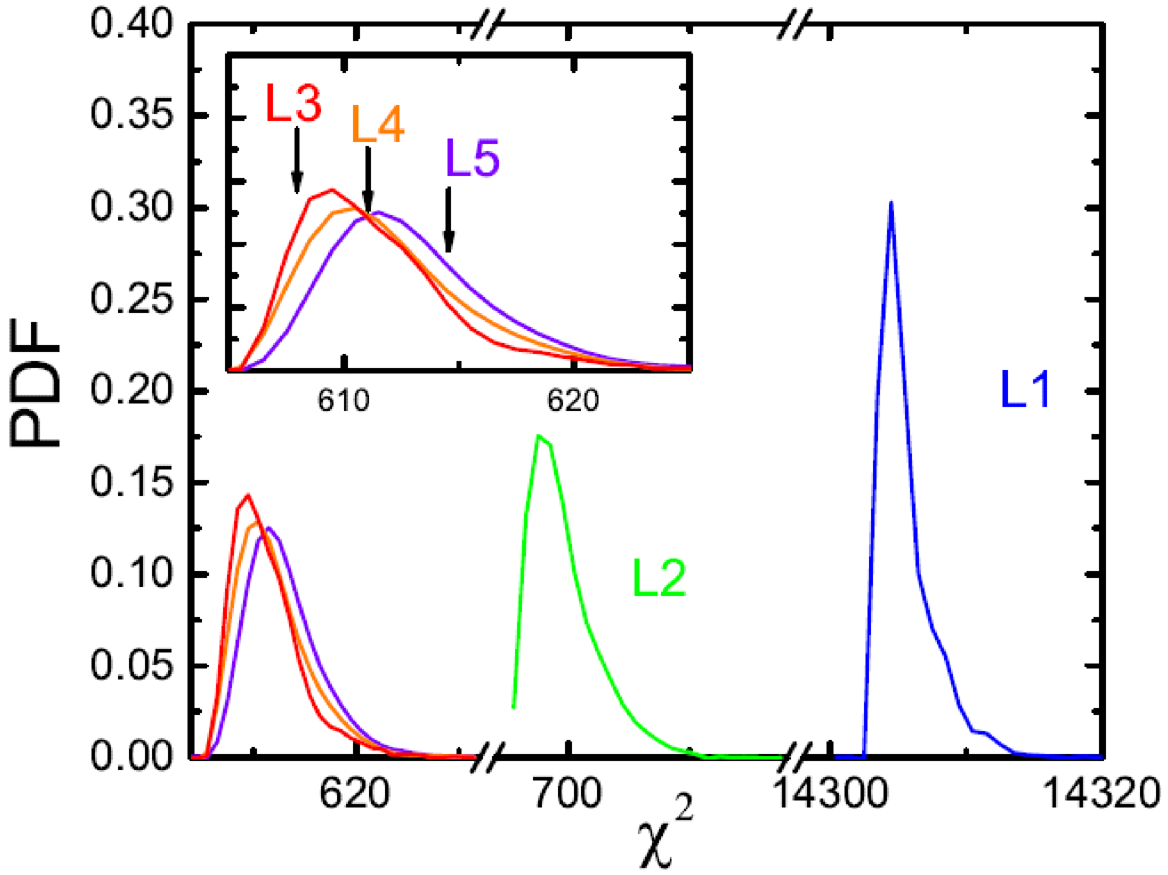
How many lines are there?

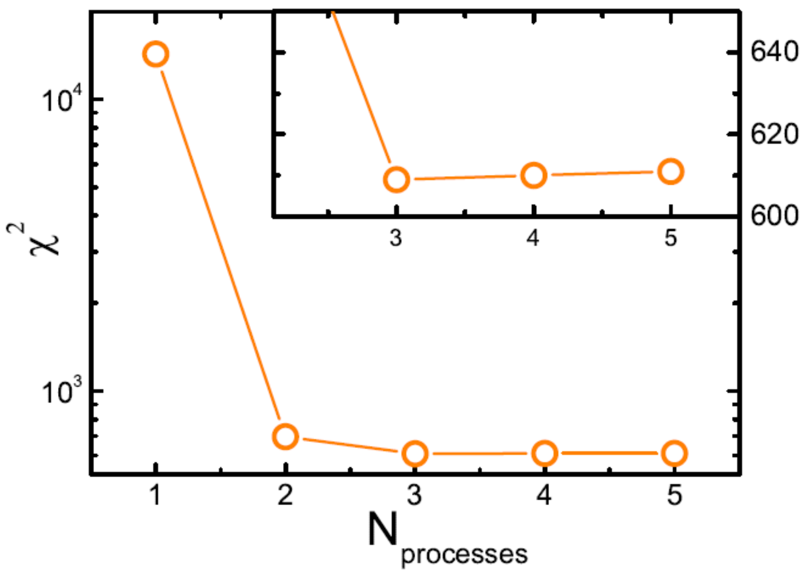
Classical model selection results

INSUFFICIENT !!!



How many lines are there?





How to use FABADA with Mantid