How does KALMAN work ?

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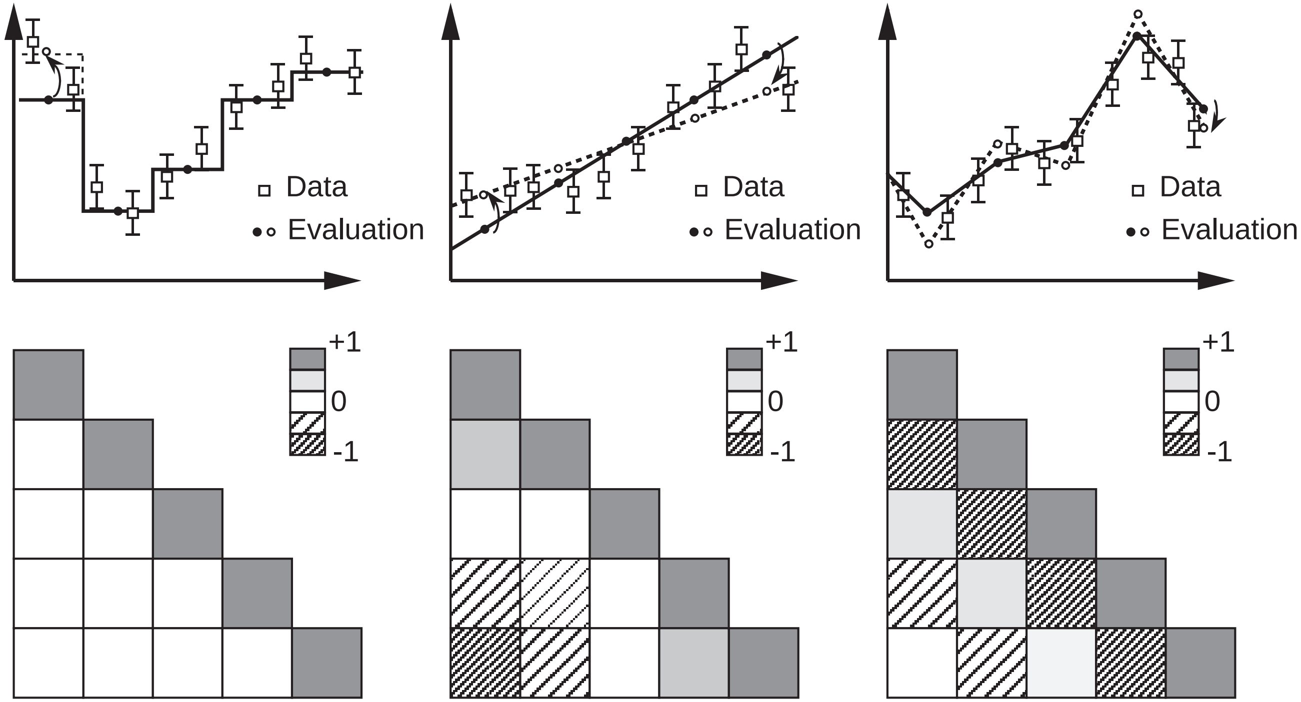
Uncertainty reduction by interpolation

- Evaluated covariance depends on the interpolation method.
  - 0-th order Spline — interval average
  - 1-st order Spline — data change smoothly like a linear function
  - function forms (model calculation) — the function describes the data tendency



The covariance matrix of evaluated quantity is a consequence of error propagation from experimental data, however those are "collapsed" data by the fitting function adopted.

KALMAN Calculation (I)

Model Parameter Fitting

- Interpolation is made with some physical background
- We believe that the mode is true
  - the fitting function is a data generation model
- Correlation exists even if experimental data are uncorrelated

Covariance Evaluation with the KALMAN code

- includes
  - Statistical / systematic errors in the experimental data
    - correlation from the systematic errors
  - Constraint by a physical model employed
    - correlation from a model which is used for interpolation
- has advantages:
  - Inter/extra-polation of uncertainties to the region where no experimental data are available
  - Covariances can be generated from an assumed parameter covariance

KALMAN Calculation (II)

Error propagation from experimental data to model parameters

$$\mathbf{P} = (\mathbf{C}^t \mathbf{V}^{-1} \mathbf{C})^{-1} \tag{1}$$

propagation from the parameters to calculated values

$$\mathbf{M} = \mathbf{C}\mathbf{P}\mathbf{C}^t \tag{2}$$

where **V**, **P**, **M** are the covariance matrices of experimental data, model parameter, and calculated values, **C** is the sensitivity matrix whose elements are $\partial f / \partial x$.

The most time-consumptive part is to construct the matrix **C**.

KALMAN Calculation (III)

Bayesian Method

$$
\begin{aligned}
x_1 &= x_0 + \mathbf{P}\mathbf{C}^t\mathbf{V}^{-1}\,(y - f(x_0)) \\
&= x_0 + \mathbf{X}\mathbf{C}^t\left(\mathbf{C}\mathbf{X}\mathbf{C}^t + \mathbf{V}\right)^{-1}(y - f(x_0)) \qquad (3) \\
\mathbf{P} &= \left(\mathbf{X}^{-1} + \mathbf{C}^t\mathbf{V}^{-1}\mathbf{C}\right)^{-1} \\
&= \mathbf{X} - \mathbf{X}\mathbf{C}^t\left(\mathbf{C}\mathbf{X}\mathbf{C}^t + \mathbf{V}\right)^{-1}\mathbf{C}\mathbf{X} \qquad (4)
\end{aligned}
$$

where x_0 and x_1 are prior / posterior vectors of the parameter, y is the experimental data vector.

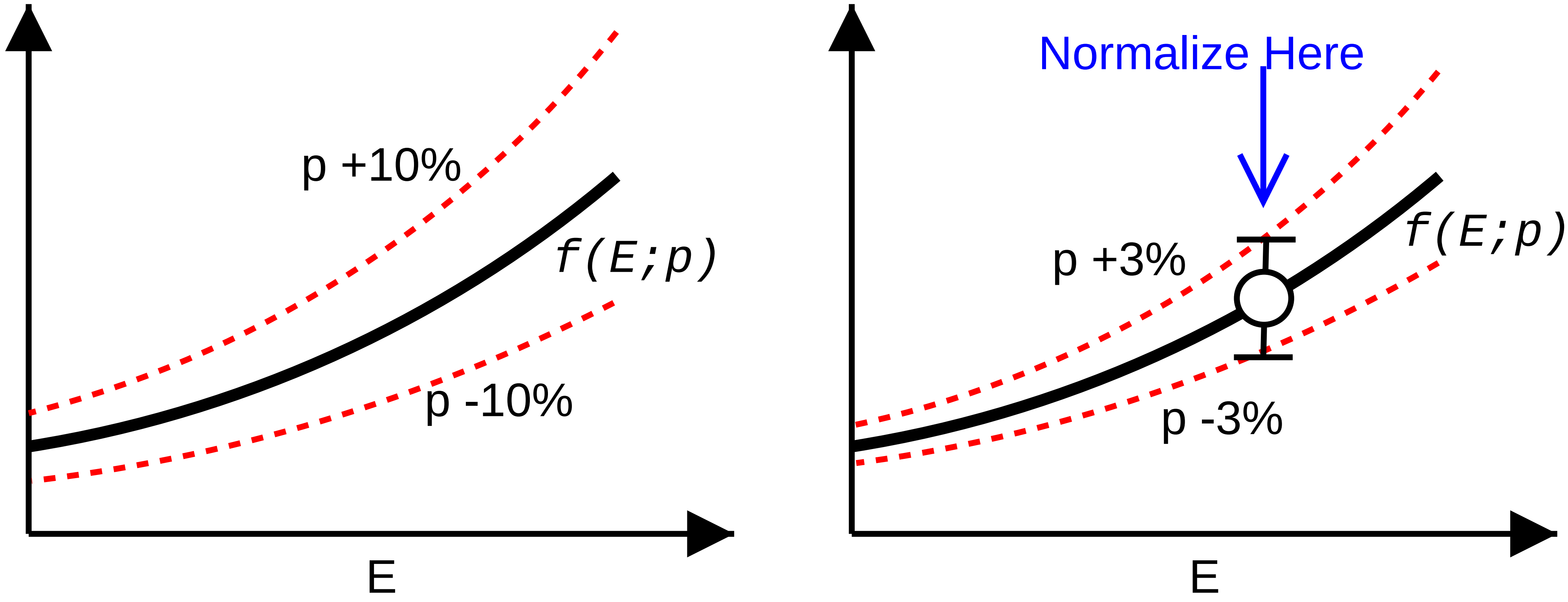
$f(x)$ is the vector which includes calculated values with the parameter x, and usually this is a non-linear function. It can be linearized by the Taylor-series expansion near x_0:

$$
y = f(x) \simeq f(x_0) + \mathbf{C}(x - x_0) \qquad (5)
$$

What we are doing ?

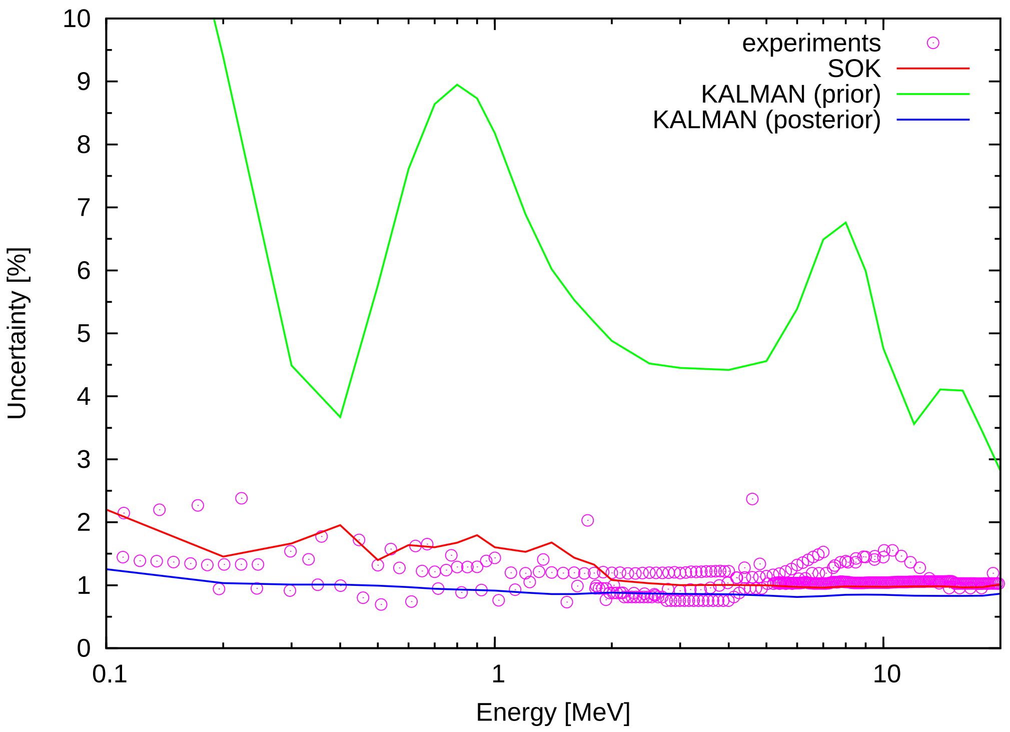
Inter/Extraporation of experimental uncertainties

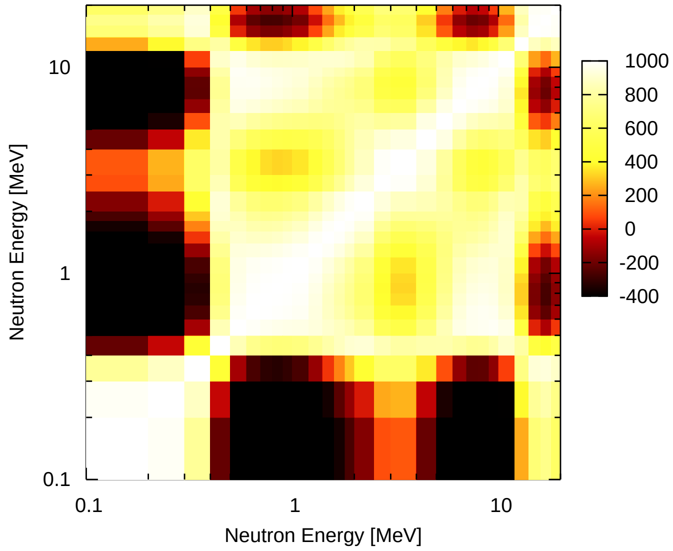
- Calculate sensitivities of model parameters
- Estimate uncertainties in the parameters by experimental data
- Calculate uncertainties in the cross sections by the parameter uncertainties

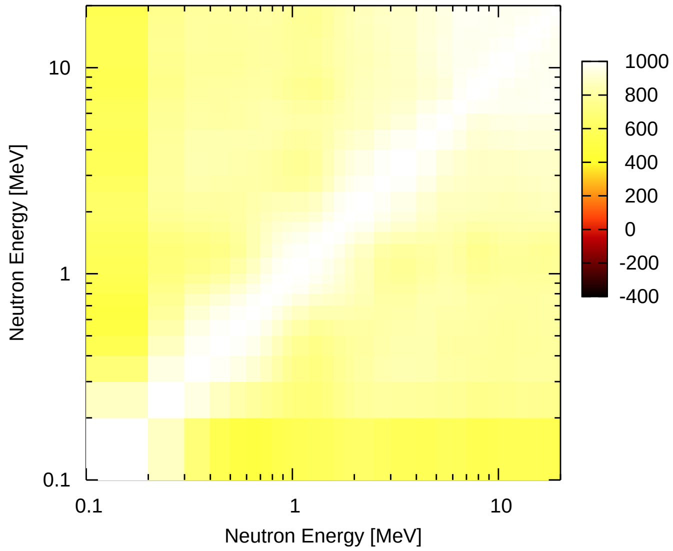


Example

Covariance for ^{232}Th total cross section







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Error Propagation (Prior Covariance)

From Model Parameters to Cross-Sections

Parameters, $p_j, 0 \le j \le M$ with uncertainties of δp_j

Observable, $(x_i, y_i), 0 \le i \le N$ with uncertainties of z_i

Our data generation model, $y = f(x; \boldsymbol{p})$

Taylor Expansion Method

$$(\delta f)^2 = \sum_j \left(\delta p_j \frac{\partial f}{\partial p_j} \right)^2 + \sum_{k \neq l} \mathrm{cov}(p_k, p_l) \frac{\partial f}{\partial p_k} \frac{\partial f}{\partial p_l}$$

Monte Carlo Method

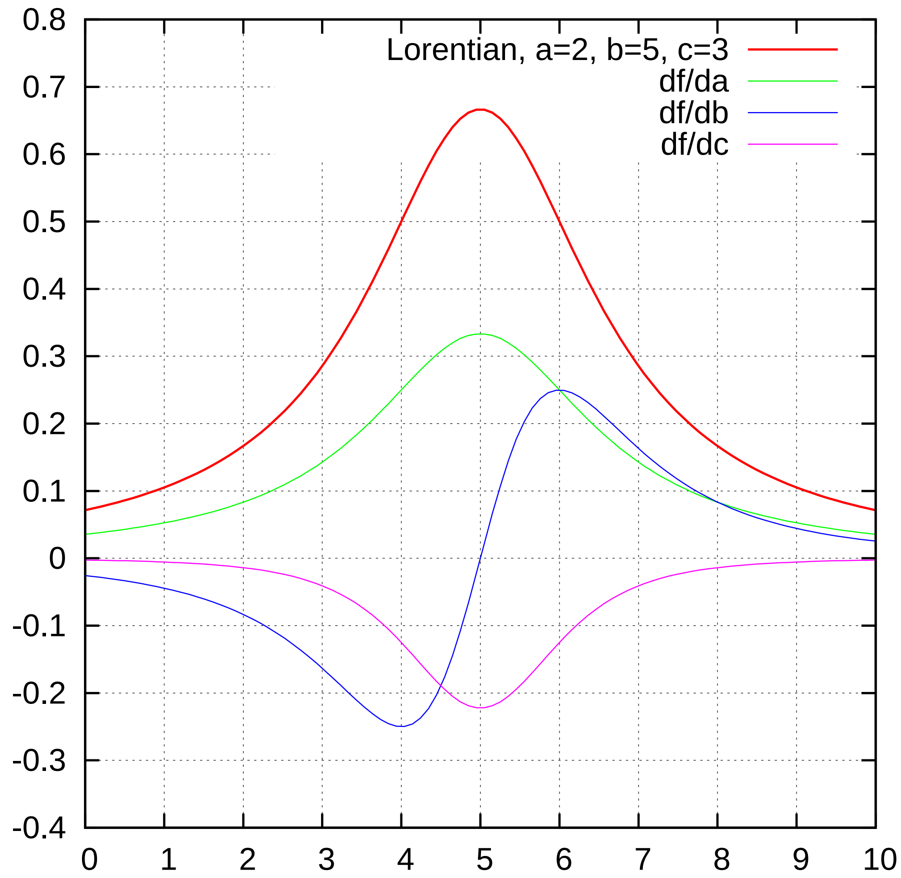
$$(\delta f)^2 = \frac{1}{K} \sum_k \left\{ f(\boldsymbol{p}^{(k)}) - f(\boldsymbol{p}^{(0)}) \right\}^2$$

Sensitivities : Taylor Expansion Method

Example — Lorentzian

$$
\begin{aligned}
f(x;a,b,c) &= \frac{a}{(x-b)^2+c} \\
\frac{\partial f}{\partial a} &= \frac{1}{(x-b)^2+c} \\
\frac{\partial f}{\partial b} &= \frac{2a(x-b)}{\left\{(x-b)^2+c\right\}^2} \\
\frac{\partial f}{\partial c} &= \frac{-a}{\left\{(x-b)^2+c\right\}^2}
\end{aligned}
$$

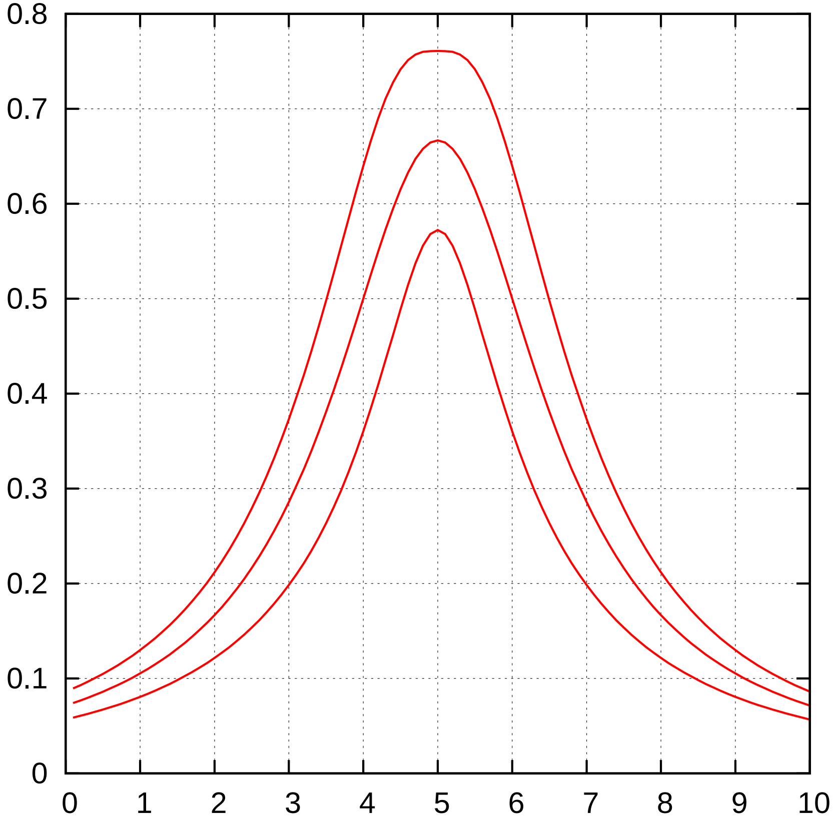
$a = 2, b = 5, c = 3$



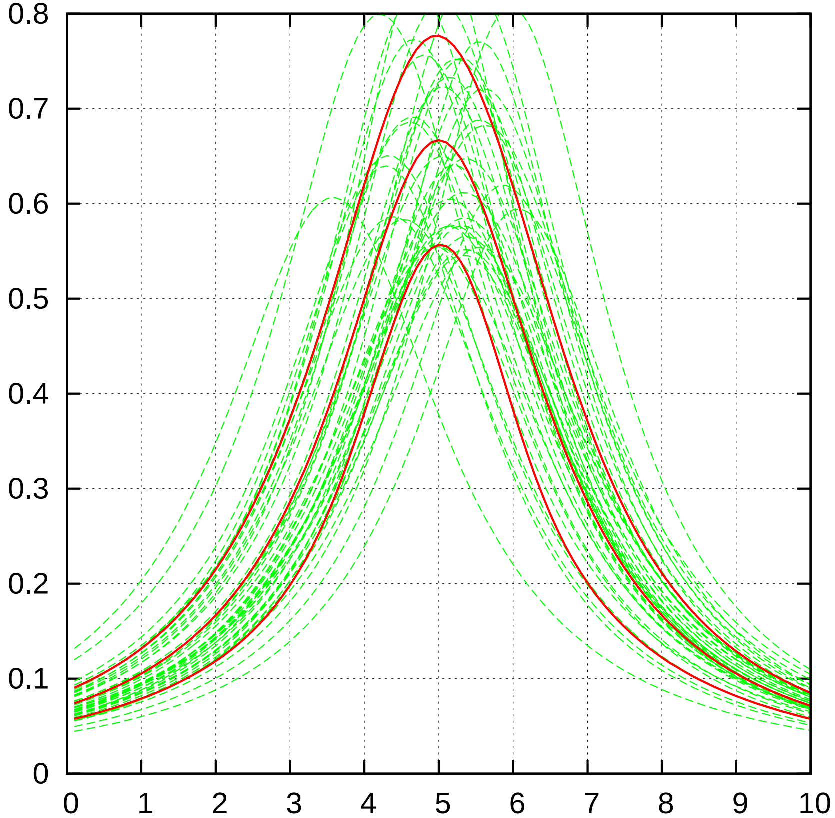
Calculated Uncertainties

Comparison of Two Methods

Taylor Expansion



Monte Carlo



10% uncertainties for each parameter without correlations are assumed.

KALMAN Method

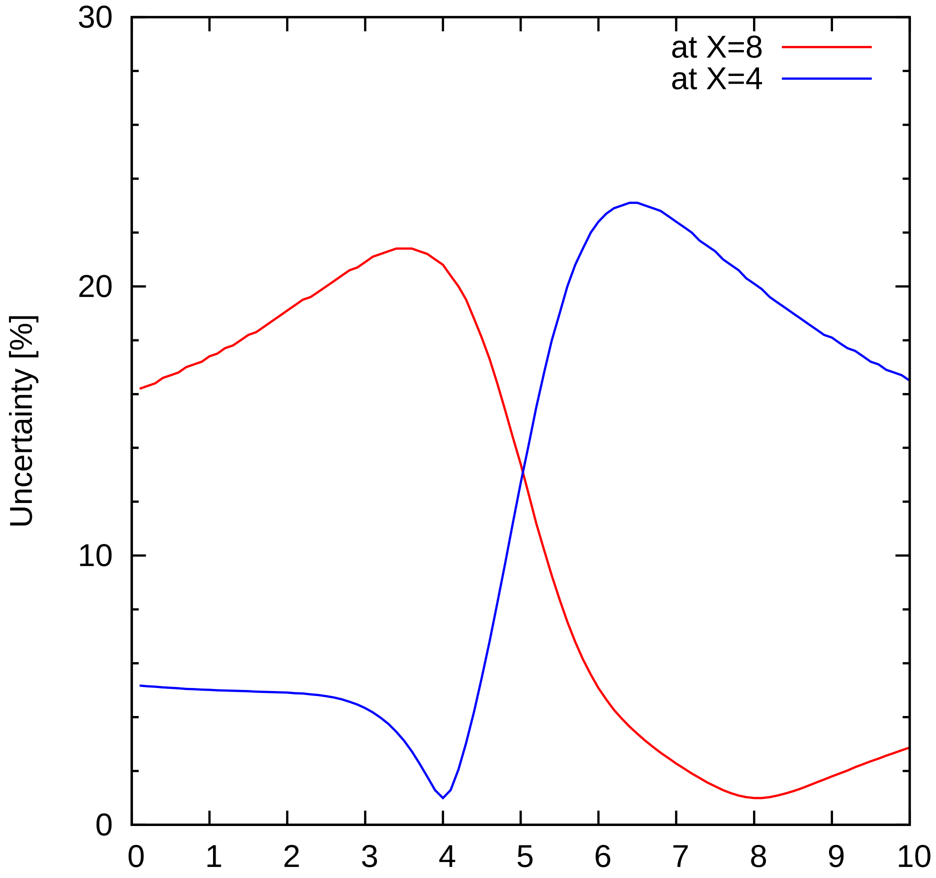
Re-normalize the Parameter Covariance

data : $y = 0.1667 \pm 1\%$ at $x = 8$

a	2.0	9.3%	100		
b	5.0	3.8%	-96	100	
c	3.0	10.0%	36	22	100

data : $y = 0.5 \pm 1\%$ at $x = 4$

a	2.0	9.3%	100		
b	5.0	4.5%	76	100	
c	3.0	9.6%	11	-55	100



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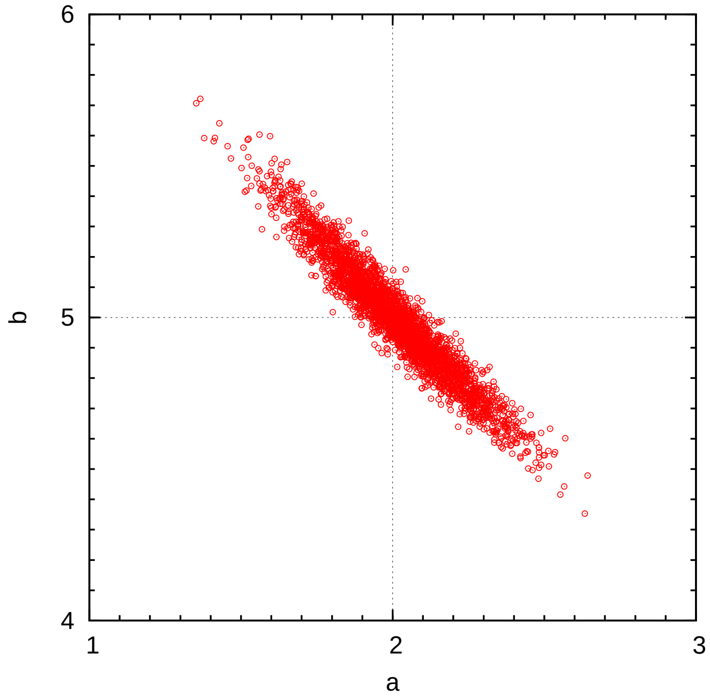
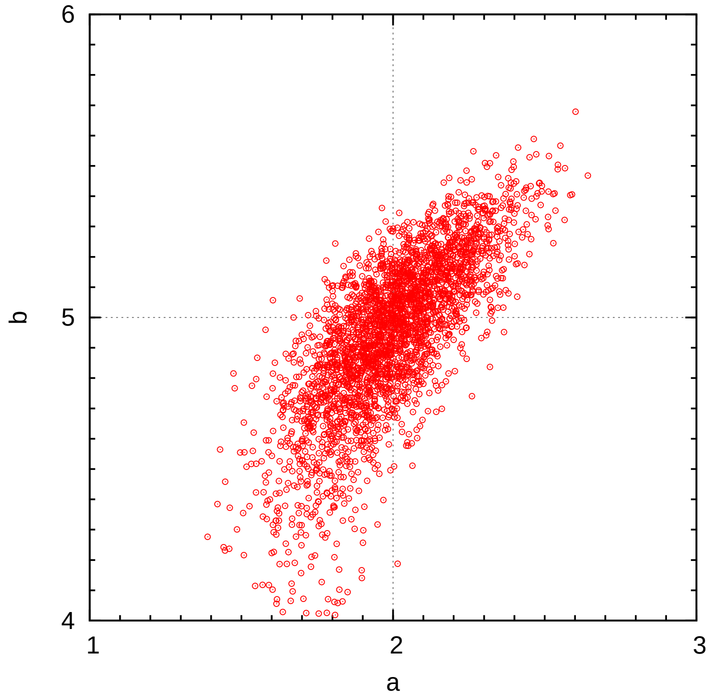
Monte-Carlo — Rejection Method

Select Parameters According to Criteria

1% at $x = 8$

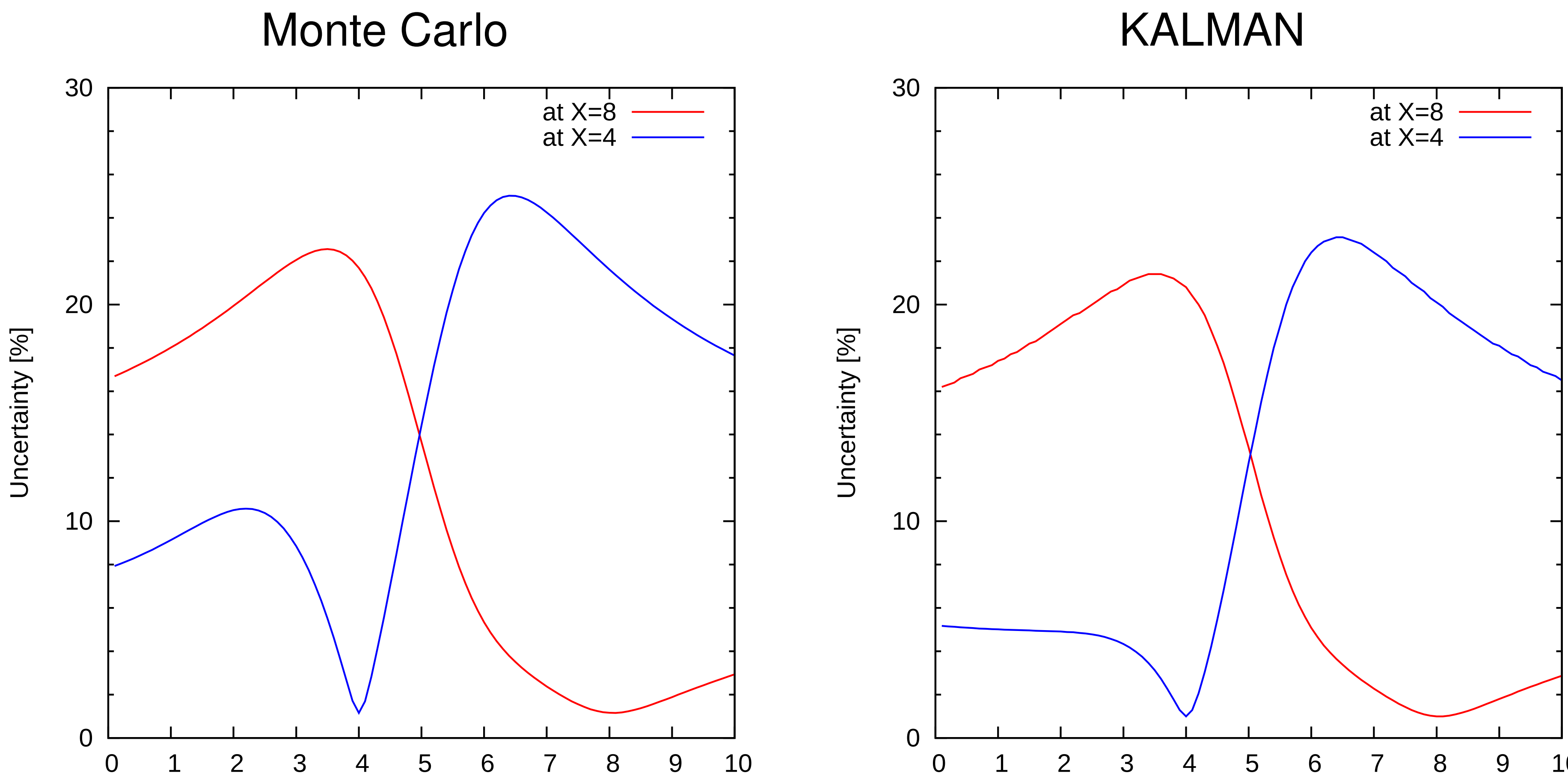


1% at $x = 4$



About 3,000 cases out of 100,000 sampled.

Uncertainties Calculated with Selected Parameters



If calculations which are larger than 1% are rejected, the unertainty minima becomes 0.57%, not 1%, because the data distribution is a Gaussian. Rejection at about 2% level gives 1% uncertainty at the minimum.

KALMAN Method — Multiple Data Points, I

Re-normalize the Parameter Covariance

no correlation

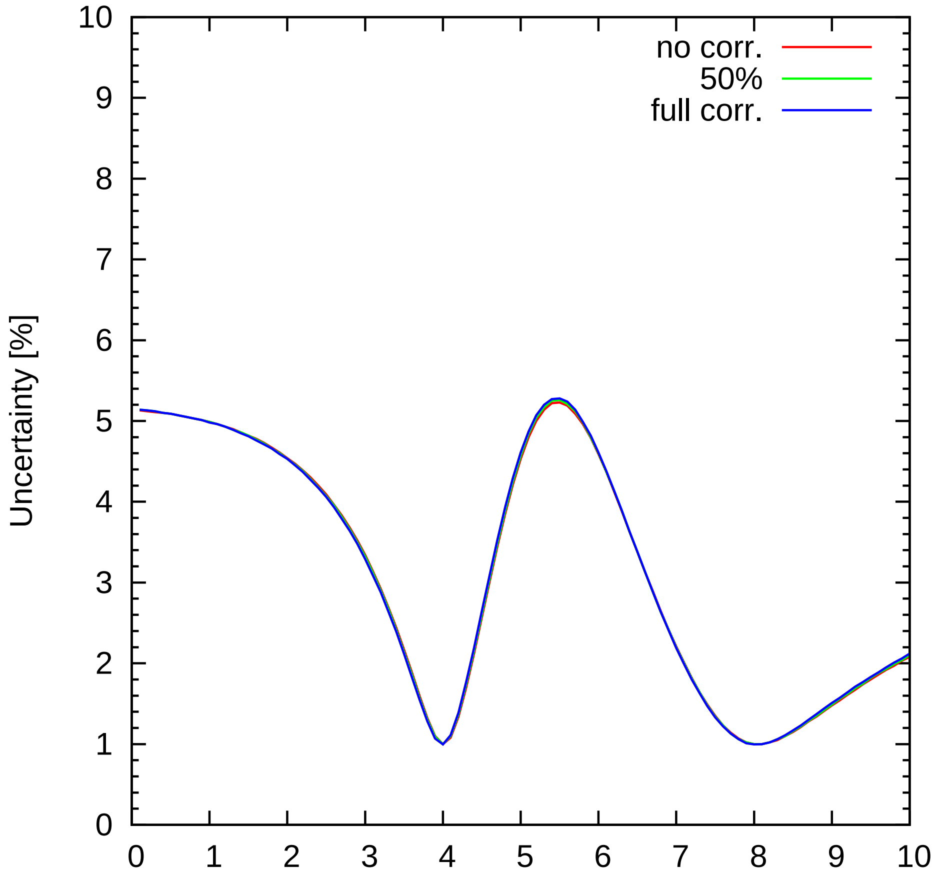
```
a 2.0  4.5%  100
b 5.0  0.9%  -94 100
c 3.0  8.9%   99 -95 100
```

50% correlation

```
a 2.0  4.5%  100
b 5.0  0.9%  -96 100
c 3.0  8.9%   98 -98 100
```

full correlation

```
a 2.0  4.5%  100
b 5.0  0.9%  -98 100
c 3.0  8.9%   98 -99 100
```



KALMAN Method — Multiple Data Points, II

More Data Points

Data at 1,2,3,= . . .,9, 1%

no correlation

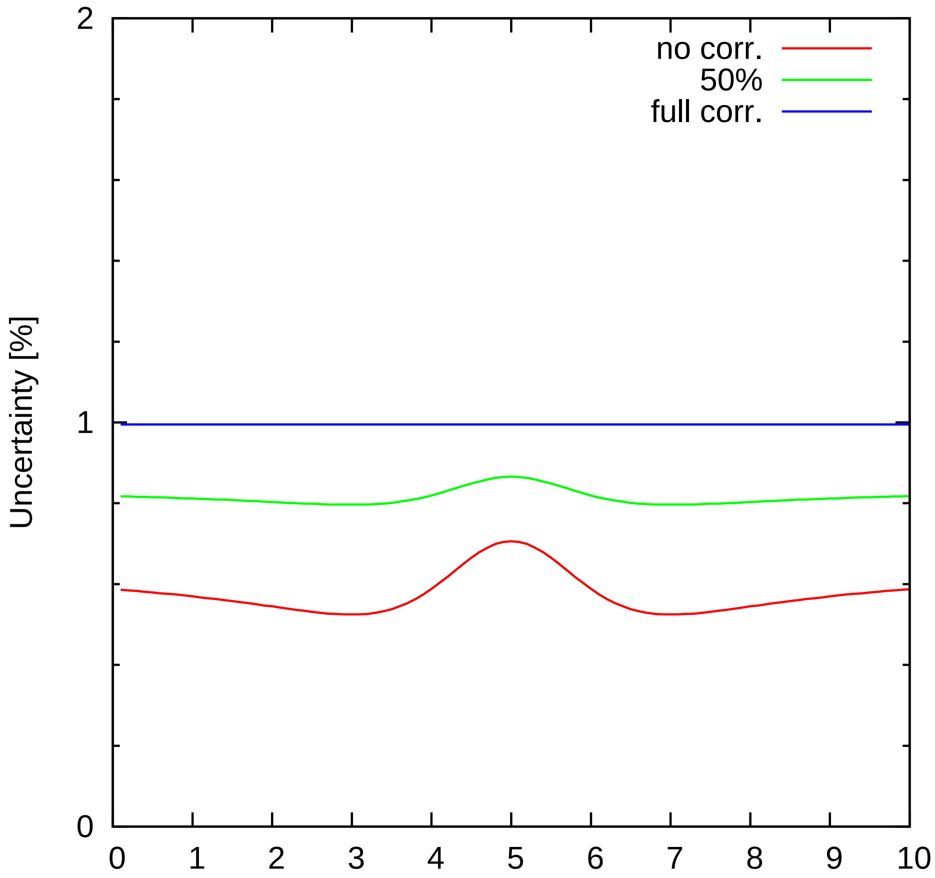
```
a 2.0  0.6%  100
b 5.0  0.1%    0 100
c 3.0  1.2%   85   0 100
```

50% correlation

```
a 2.0  0.8%  100
b 5.0  0.1%    0 100
c 3.0  0.8%   45   0 100
```

full correlation

```
a 2.0  1.0%    100
b 5.0  0.004%    0 100
c 3.0  0.4%      2   0 100
```



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Parameter Space $\longleftrightarrow$ Data Space

KALMAN Method

Parameter Space
p; **X**
$\mathbf{P} = \left(\mathbf{X}^{-1} + \mathbf{C}^t\mathbf{V}^{-1}\mathbf{C}\right)^{-1}$

Observable Space
σ; **V**
$\mathbf{M} = \mathbf{CPC}^t$

Monte-Carlo Method in the Data Space

Parameter Space
p; **X**

Observable Space
σ; **V**
W from MC wtih assumed **X**, or
$\mathbf{M} = \left(\mathbf{W}^{-1} + \mathbf{V}^{-1}\right)^{-1}$

Backward-Forward Monte-Carlo Method (E.Bauge)

Parameter Space
p; uniform

Observable Space
σ; **V**
W from MC
calculate χ_i^2 for each sampled p_i
weighing average, $w_i = f(\chi_i^2) \rightarrow \mathbf{X}$

p; **X**

M from MC wtih **X**

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