



**International Atomic Energy Agency**

## **Evaluation: Least Squares and Weighted Mean**

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# Various Evaluation Methodology

Evaluation methodology depends on availability of experimental data and model:

- Eye-guide: Historical approach, *no longer acceptable....*
- Least-squares fitting to experimental data  
(e.g., fission cross sections for standards)
- Model calculation
- Mixture of experimental data and model calculation data  
(e.g., Unified Monte Carlo approach UMC–Capote+Smith).



## Model and Model Parameter

Adjustment of model parameters  $\mathbf{p}$  to reproduce experimental data  $\mathbf{y}$  is often an essential part of data evaluation, for example

- Optical potential parameters to reproduce experimental (total) reaction cross sections.
- Fission barrier parameters to reproduce experimental fission cross sections.
- Fission neutron multiplicities to reproduce experimental k-eff.
- Evaluated cross section to reproduce experimental cross section.

Model parameters  $\mathbf{p}$  and experimental data  $\mathbf{y}$  are related by a model  $\mathbf{f}$ :  $\mathbf{y}=\mathbf{f}(\mathbf{p})+\Delta$  (or  $\mathbf{y}\sim\mathbf{f}(\mathbf{p})$ ).

The model  $\mathbf{f}$  does not always have analytical expression. (e.g., input and output of reaction model codes).



# Conventional Least Squares

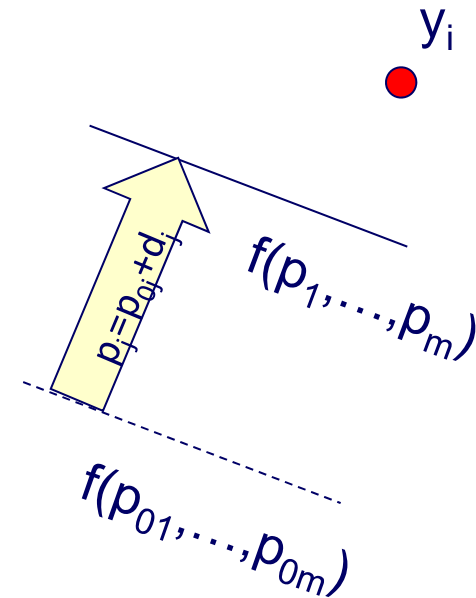
## Problem:

1. There is an old model parameter set  $p_{0j}$  ( $j=1,m$ ) which is related with experimental observable by the fitting function  $f$ :

$$f_i(p_{01}, \dots, p_{0m}) .$$

2. New experimental data points  $y_i$  ( $i=1,n$ ) are available.

3. We want to have an updated new model parameter set  $p_j$  ( $j=1,m$ ) by using new experimental data points  $y_i$  ( $i=1,n$ ).



# Minimize Chi-Square

Difference between in new and old model parameters:

$$p_j = p_{0j} + d_j \quad (j=1, m).$$

This makes the following change in  $f_i(p_1, \dots, p_m)$ :

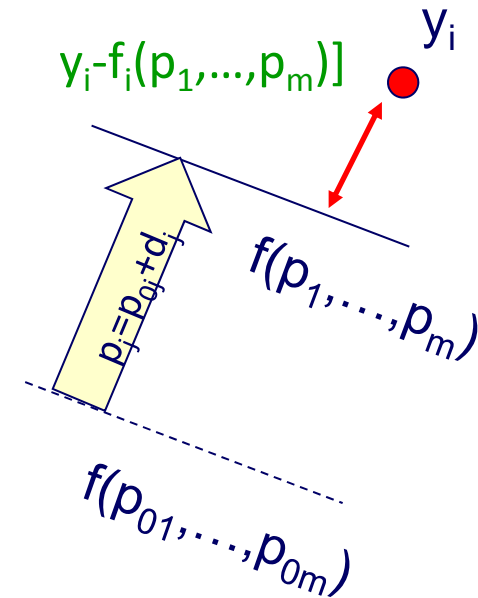
$$f_i(p_1, \dots, p_m) \sim f_i(p_{01}, \dots, p_{0m}) + \sum_{j=1, m} a_{ij} \cdot d_j$$

$$\text{with } a_{ij} = \left. \frac{\partial f_i}{\partial p_j} \right|_{p=p_0}.$$

$d_j$  must be chosen so that the sum of deviation between  $y_i$  and  $f_i(p_1, \dots, p_m)$  is minimum:

$$\chi^2 = Q(d_1, \dots, d_m) = \sum_{i=1, n} [y_i - f_i(p_1, \dots, p_m)]^2 = \text{Min.}$$

if we trust all experimental points by the same weight.



old mod. param.  $p_{0j}$  ( $j=1, m$ ), updated mod. param.  $p_j$  ( $j=1, m$ )  
 new exp. points  $y_i$  ( $i=1, n$ ), model  $f: y \sim f(p)$



## Minimum Condition Weighted by Variance

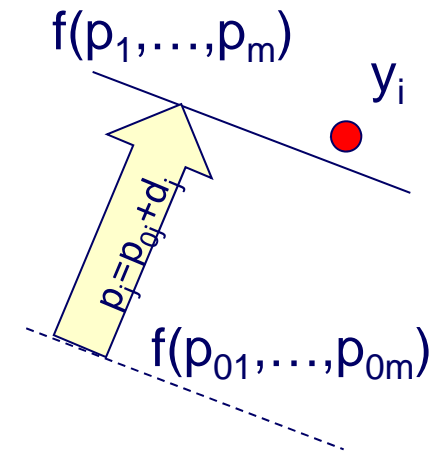
The minimum condition

$$Q(d_1, \dots, d_m) = \sum_{i=1, n} [y_i - f_i(p_1, \dots, p_m)]^2 = \text{Min.}$$

is revised to

$$Q(d_1, \dots, d_m) = \sum_{i=1, n} [y_i - f_i(p_1, \dots, p_m)]^2 / (\Delta y_i)^2 = \text{Min.}$$

if each experimental point  $y_i$  has its standard deviation  $\Delta y_i = (V_{ii})^{1/2}$ .



This minimum condition gives m equations:

$$\partial Q(d_1, \dots, d_m) / \partial d_i = 0 \quad (i=1, m).$$

old mod. param.  $p_{0j}$  ( $j=1, m$ ), updated mod. param.  $p_j$  ( $j=1, m$ )  
new exp. points  $y_i$  ( $i=1, n$ ), model  $f: y \sim f(p)$



## Equations for Parameter Shift $p - p_0$

$$Q(d_1, \dots, d_m) = \sum_{i=1, n} [y_i - f_i(p_1, \dots, p_m)]^2 / V_{ii} = \text{Min.}$$

$$\rightarrow \partial Q(d_1, \dots, d_m) / \partial d_j = 0 \quad (j=1, m).$$

$$\rightarrow \partial Q(d_1, \dots, d_m) / \partial d_j = \left\{ \sum_{i=1, n} 2[y_i - f_i(p_1, \dots, p_m)] / V_{ii} \right\} (\partial f_i / \partial d_j) = 0$$

$$\left\{ \sum_{i=1, n} [y_i - f_i(p_1, \dots, p_m)]^2 / V_{ii} \right\} \cdot \underline{(\partial f_i / \partial d_j)} = 0 \quad (j=1, m) \quad (*)$$

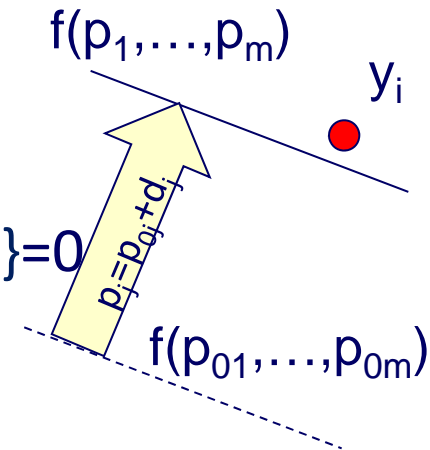
Recalling the linear expansion,

$$f_i(p_1, \dots, p_m) \sim f_i(p_{01}, \dots, p_{0m}) + \sum_{j=1, m} a_{ij} \cdot d_j \quad \text{with } a_{ij} = \partial f_i / \partial p_j |_{p=p_0} \quad (j=1, m),$$

we obtain  $(\partial f_i / \partial d_j) = a_{ij}$ .

By putting this relation to (\*),

$$\sum_{i=1, n} [y_i - f_i(p_{01}, \dots, p_{0m}) - \sum_{k=1, m} a_{ik} \cdot d_k] a_{ij} / V_{ii} = 0 \quad (j=1, m). \quad (\text{normal eq.})$$



old mod. param.  $p_{0j}$  ( $j=1, m$ ), updated mod. param.  $p_j$  ( $j=1, m$ )  
 new exp. points  $y_i$  ( $i=1, n$ ), model  $f: y \sim f(p)$



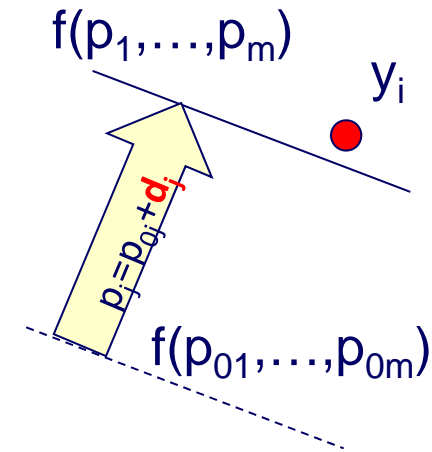
# Normal Equation

$$Q(d_1, \dots, d_m) = \sum_{i=1, n} [y_i - f_i(p_1, \dots, p_m)]^2 / V_{ii} = \min.$$

→

$$\sum_{i=1, n} [y_i - f_i(p_{01}, \dots, p_{0m}) - \sum_{k=1, m} a_{ik} \cdot d_k] a_{ij} / V_{ii} = 0 \quad (j=1, m).$$

with  $a_{ij} = \partial f_i / \partial p_j |_{p=p_0}$ .



We obtain  $m$  equations for  $d_j$  ( $j=1, m$ ) – “Normal equation”.

All  $y_i$ ,  $V_{ii}$ ,  $a_{ij}$ ,  $p_{0j}$  are known with the analytical form of  $f_i$  ( $i=1, n$ ;  $j=1, m$ ), and we can solve these equations for  $d_j$  ( $j=1, m$ ) which minimize  $Q(d_1, \dots, d_m)$ .

old mod. param.  $p_{0j}$  ( $j=1, m$ ), updated mod. param.  $p_j$  ( $j=1, m$ )  
new exp. points  $y_i$  ( $i=1, n$ ), model  $f: y \sim f(p)$





## Conventional Least Squares

$$\sum_{i=1,n} (a_{ij}/V_{ii}) [y_i - f_i(p_{01}, \dots, p_{0m}) - \sum_{k=1,m} a_{ik} \cdot d_k] = 0 \quad (j=1,m).$$

with  $a_{ij} = \partial f_i / \partial p_j |_{p=p_0}$ ,  $d_k = p_k - p_{0k}$

Let us introduce the following vector/matrix notation:

$\mathbf{y} = \{y_i\}$ ,  $\mathbf{y}_0 = \{f_i(p_{01}, \dots, p_{0m})\}$  (n dimensional vectors)

$\mathbf{p} = \{p_j\}$ ,  $\mathbf{p}_0 = \{p_{0j}\}$  (m dimensional vectors)

$\mathbf{G} = \{a_{ij}\}$  (n × m matrix),  $\mathbf{V}^{-1} = \{1/V_{ii}\}$  (n × n diagonal matrix)

, then  $\mathbf{G}^t \mathbf{V}^{-1} [\mathbf{y} - \mathbf{y}_0 - \mathbf{G}(\mathbf{p} - \mathbf{p}_0)] = 0$ .

This gives the updated fitting parameters  $\mathbf{p} = \{p_j\}$ :

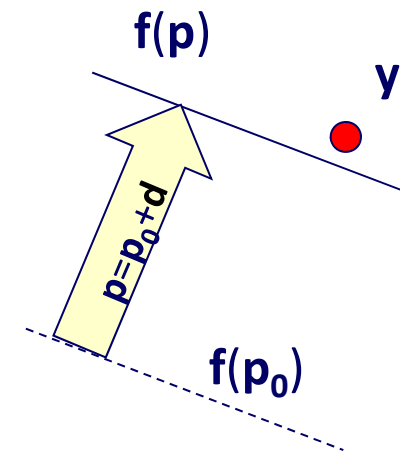
$$\mathbf{p} = \mathbf{p}_0 + (\mathbf{G}^t \mathbf{V}^{-1} \mathbf{G})^{-1} \mathbf{G}^t \mathbf{V}^{-1} (\mathbf{y} - \mathbf{y}_0)$$

old mod. param.  $p_{0j}$  (j=1,m), updated mod. param.  $p_j$  (j=1,m)  
new exp. points  $y_i$  (i=1,n), model  $f: y \sim f(p)$



## What We Solved??

1. Default parameter  $\mathbf{p}_0$  for model  $\mathbf{f}$
2. New experimental data  $\mathbf{y}$
3. The parameter  $\mathbf{p}_0$  describe  $\mathbf{y}$  by  $\mathbf{f}(\mathbf{p}_0)$
4. Find  $\mathbf{p}$  which minimize “distance” between  $\mathbf{y}$  and  $\mathbf{f}(\mathbf{p})$ .



$$\rightarrow \mathbf{p} = \mathbf{p}_0 + (\mathbf{G}^t \mathbf{V}^{-1} \mathbf{G})^{-1} \mathbf{G}^t \mathbf{V}^{-1} (\mathbf{y} - \mathbf{y}_0)$$



## Covariance of New Model Parameters $\mathbf{p}$

Updated model parameter  $\mathbf{p}$  for experimental points  $\mathbf{y} \sim \mathbf{f}(\mathbf{p})$

$$\mathbf{p} = \mathbf{p}_0 + (\mathbf{G}^t \mathbf{V}^{-1} \mathbf{G})^{-1} \mathbf{G}^t \mathbf{V}^{-1} (\mathbf{y} - \mathbf{y}_0)$$

If we define  $\mathbf{K} = (\mathbf{G}^t \mathbf{V}^{-1} \mathbf{G})^{-1} \mathbf{G}^t \mathbf{V}^{-1}$ ,  $\mathbf{p} = \mathbf{p}_0 + \mathbf{K}(\mathbf{y} - \mathbf{y}_0)$  or  $p_f = p_{0f} + \sum_{i=1, m} K_{fi} (y_i - y_{0i})$

For two linear combinations  $f = \sum_{i=1, n} K_{fi} y_i$  and  $g = \sum_{j=1, m} K_{gj} y_j$ ,

The covariance between  $f$  and  $g$  is

$$V_{fg} = \sum_{i=1, n; j=1, m} K_{fi} K_{gj} V_{ij} \quad (V_{ij}: \text{covariance between } y_i \text{ and } y_j).$$

Therefore the covariance between  $p_f$  and  $p_g$  is

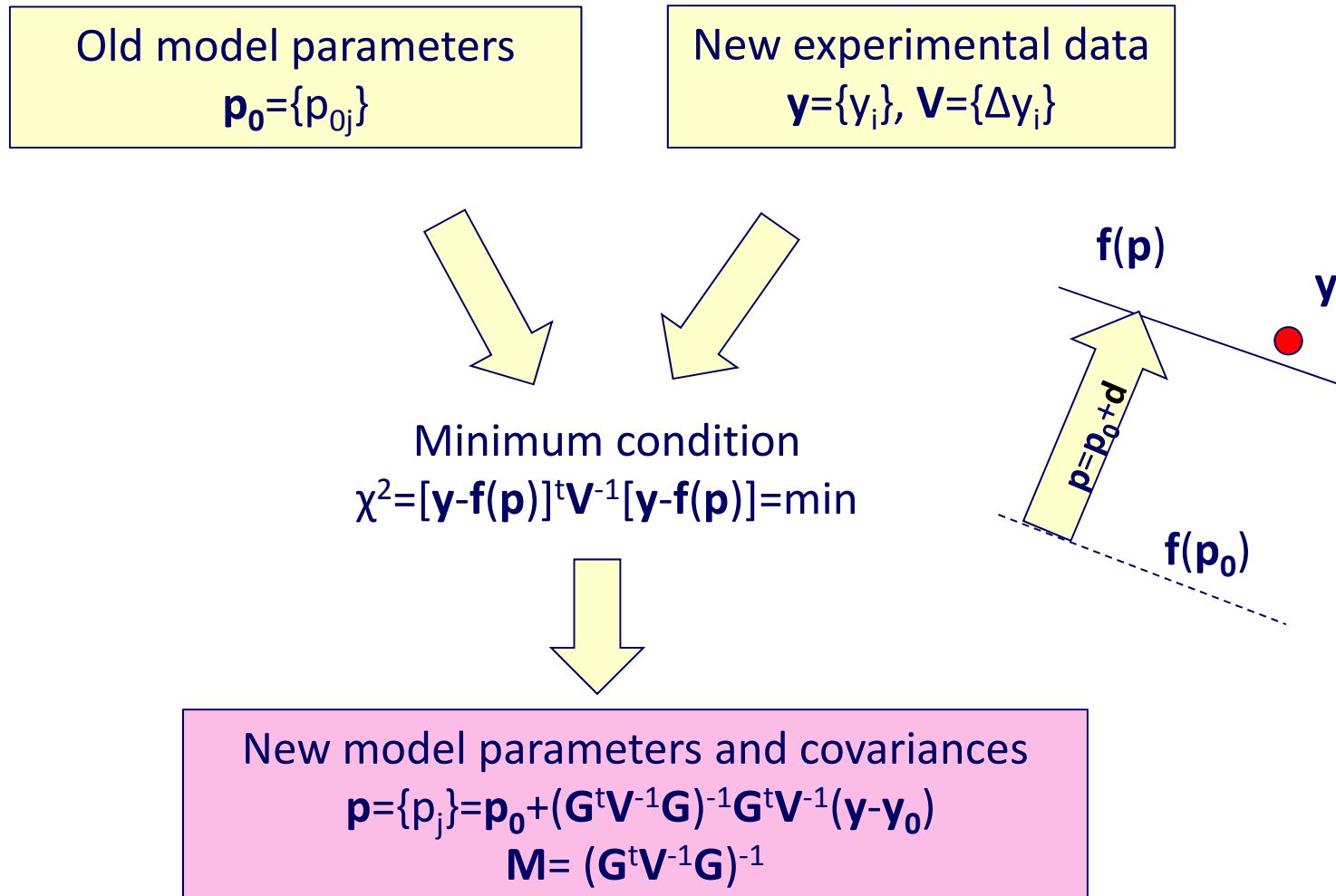
$$M_{fg} = \sum_{i=1, n; j=1, m} K_{fi} K_{gj} V_{ij} \quad \text{or}$$

$$\mathbf{M} = \mathbf{K} \mathbf{V} \mathbf{K}^t = [(\mathbf{G}^t \mathbf{V}^{-1} \mathbf{G})^{-1} \mathbf{G}^t \mathbf{V}^{-1}] \mathbf{V} [(\mathbf{G}^t \mathbf{V}^{-1} \mathbf{G})^{-1} \mathbf{G}^t \mathbf{V}^{-1}]^t = (\mathbf{G}^t \mathbf{V}^{-1} \mathbf{G})^{-1}$$

$$\mathbf{p} = \sum_{i=1, n} a_i \cdot x_i \rightarrow V_{pq} \sim \sum_{i=1, n; j=1, m} g_i h_j V_{ij} \quad g_i = (\partial p / \partial x_i)_{x_i = \langle x_i \rangle}, \quad h_j = (\partial q / \partial y_j)_{y_j = \langle y_j \rangle}$$

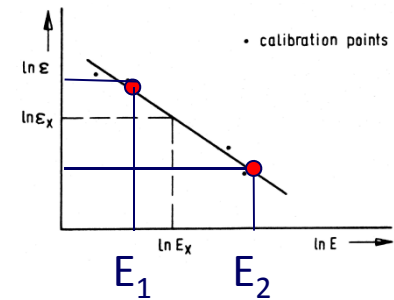


# Flow of Conventional Least Squares



# Adjustment Makes Correlation between Parameters!

Adjustment to experimental points  $\mathbf{y}$  creates correlation  $\mathbf{M}$  between model parameters  $\mathbf{p}$ !



## Example: Efficiency curve $\varepsilon=f(\mathbf{p})$

Model (fitting) parameters  $\mathbf{p}$  were determined to reproduce efficiency values at several calibration points by standard sources.

Even if these calibration points are independent each other,  $\mathbf{p}$  gets correlation  $\mathbf{M}$ .

Efficiencies at two energies interpolated by the model (fitting)  $\varepsilon_1=f(E_1,\mathbf{p})$  and  $\varepsilon_2=f(E_2,\mathbf{p})$  are also correlated through  $\mathbf{M}$ .



# Weighted Average

## Conventional least squares:

n experimental points  $y_i \pm \Delta y_i$ ,  $v_{ii} = \Delta y_i^2$ ,  $(V_{ii})^{1/2} = \Delta y_i$  ( $i=1, n$ )

→ find  $p_j$  ( $j=1, m$ ) which minimize  $\sum_{i=1, n} [y_i - f_i(p_1, \dots, p_m)]^2 / V_{ii}$ .

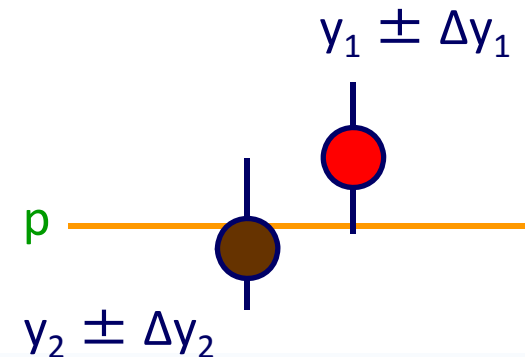
## Weighted average p of experimental points $y_1$ and $y_2$ :

2 experimental points  $y_1 \pm \Delta y_1$  and  $y_2 \pm \Delta y_2$ ,  $v_{11} = \Delta y_1^2$  and  $v_{22} = \Delta y_2^2$ .

→ find p which minimize  $Q = \chi^2 = (y_1 - p)^2 / V_{11} + (y_2 - p)^2 / V_{22}$

→  $\partial Q / \partial p = 0$

→  $p = [(y_1 / V_{11}) + (y_2 / V_{22})] / [(1 / V_{11}) + (1 / V_{22})]$



## Weighted Average

From 2 experiment x-sections  $y_1 \pm \Delta y_1$  and  $y_2 \pm \Delta y_2$ .

$$p = [(y_1/V_{11}) + (y_2/V_{22})] / [(1/V_{11}) + (1/V_{22})]$$
$$= [(y_1/\Delta y_1^2) + (y_2/\Delta y_2^2)] / [(1/\Delta y_1^2) + (1/\Delta y_2^2)]$$

If we define  $w_1 = 1/\Delta y_1^2$  and  $w_2 = 1/\Delta y_2^2$ , this equation becomes

$$p = (w_1 y_1 + w_2 y_2) / (w_1 + w_2)$$

This is a linear combination of  $y_1$  and  $y_2$ , and therefore

$$(\Delta p)^2 = M_{pp} = [w_1 / (w_1 + w_2)] \Delta y_1^2 + [w_2 / (w_1 + w_2)] \Delta y_2^2$$
$$= \Delta y_1^2 \Delta y_2^2 / (\Delta y_1^2 + \Delta y_2^2)$$

This is the **weighted average** of two experimental data points which have variances without correlation.

$$p = \sum_{i=1,n} a_i \cdot x_i \rightarrow \langle p \rangle = \sum_{i=1,n} a_i \langle x_i \rangle, V_{pp} = \langle p^2 \rangle - \langle p \rangle^2 = \sum_{i=1,n} a_i^2 V_{ii} + 2 \sum_{i=1,n; j=1,n; i < j} a_i a_j V_{ij}$$



## Example of Weighted Average

**Weighted average:**

$$y_1 \pm \Delta y_1, y_2 \pm \Delta y_2$$

$$\rightarrow p = [(y_1/\Delta y_1^2) + (y_2/\Delta y_2^2)] / [(1/\Delta y_1^2) + (1/\Delta y_2^2)],$$

$$(\Delta p)^2 = \Delta y_1^2 \Delta y_2^2 / (\Delta y_1^2 + \Delta y_2^2)$$

**Example (Exercise):**

Calculate the weighted average and its standard deviation for

$$y_1 \pm \Delta y_1 = \mathbf{1.0 \pm 0.1} \text{ and } y_2 \pm \Delta y_2 = \mathbf{1.2 \pm 0.2}$$

Weighted average:

$$p = [(1.0/0.1^2) + (1.2/0.2^2)] / [(1/0.1^2) + (1/0.2^2)] = \mathbf{1.04}.$$

Variance:

$$(\Delta p)^2 = (0.1^2 \cdot 0.2^2) / (0.1^2 + 0.2^2) = 0.008 \quad \Delta p = \mathbf{0.089}.$$





# Off-Diagonal Weighted Average

## Conventional least squares:

n experimental points  $y_i \pm \Delta y_i$ ,  $v_{ii} = \Delta y_i^2$ ,  $(v_{ii})^{1/2} = \Delta y_i$  ( $i=1, n$ )

→ find  $p_j$  ( $j=1, m$ ) minimizing  $\sum_{i=1, n} [y_i - f_i(p_1, \dots, p_m)]^2 / V_{ii}$

or  $[\mathbf{y} - \mathbf{f}(\mathbf{p})]^t \mathbf{V}^{-1} [\mathbf{y} - \mathbf{f}(\mathbf{p})]$  in vector-matrix notation.

This expression is valid also when  $\mathbf{V}$  has off-diagonal elements.

## Off-diagonal weighted average $p$ of experimental points $y_1$ and $y_2$ :

2 experimental points  $y_1 \pm \Delta y_1$  and  $y_2 \pm \Delta y_2$  with covariance  $\mathbf{V}$ .

→ find  $p$  minimizing  $Q = \chi^2 = [\mathbf{y} - \mathbf{f}(p)]^t \mathbf{V}^{-1} [\mathbf{y} - \mathbf{f}(p)] = \sum_{i,j=1,2} (y_i - p) V^{-1}_{ij} (y_j - p)$

→  $\partial Q / \partial p = 0 \rightarrow \dots \rightarrow \mathbf{p} = [(\mathbf{V}_{22} - \mathbf{V}_{12})y_1 + (\mathbf{V}_{11} - \mathbf{V}_{12})y_2] / (\mathbf{V}_{11} + \mathbf{V}_{22} - 2\mathbf{V}_{12})$

This is the **weighted average** of two experimental data points which have covariance (with correlation).



## Variance of Off-Diagonal Weighted Average

Off-diagonal weighted average of  $y_1$  and  $y_2$ :

$$p = [(V_{22}-V_{12})y_1 + (V_{11}-V_{12})y_2] / (V_{11}+V_{22}-2V_{12})$$

If we set  $a = (V_{22}-V_{12}) / (V_{11}+V_{22}-2V_{12})$  and  $b = (V_{11}-V_{12}) / (V_{11}+V_{22}-2V_{12})$ ,

$p = (ay_1 + by_2)$  – linear combination of  $y_1$  and  $y_2$ .

Applying the error propagation law for linear combination,

$$\begin{aligned} (\Delta p)^2 = v_{pp} &= a^2 V_{11} + b^2 V_{22} + 2ab V_{12} \\ &= [(V_{22}-V_{12})^2 V_{11} + (V_{11}-V_{12})^2 V_{22} + 2(V_{22}-V_{12})(V_{11}-V_{12})V_{12}] \\ &\quad / (V_{11}+V_{22}-2V_{12})^2. \\ &= [V_{11}V_{22} - (V_{12})^2] / (V_{11}+V_{22}-2V_{12}) \end{aligned}$$

$$p = \sum_{i=1,n} a_i \cdot x_i \rightarrow \langle p \rangle = \sum_{i=1,n} a_i \langle x_i \rangle, \quad v_{pp} = \langle p^2 \rangle - \langle p \rangle^2 = \sum_{i=1,n} a_i^2 V_{ii} + 2 \sum_{i=1,n; j=1,n; i < j} a_i a_j V_{ij}$$



## Diagonal and Off-Diagonal Weighted Average

### Off-diagonal weighted average

$$\rho = [(V_{22} - V_{12})y_1 + (V_{11} - V_{12})y_2] / (V_{11} + V_{22} - 2V_{12})$$

$$(\Delta\rho)^2 = [V_{11}V_{22} - (V_{12})^2] / (V_{11} + V_{22} - 2V_{12})$$

If we set  $V_{12} = 0$ , then we obtain

$$\rho = [V_{22}y_1 + V_{11}y_2] / (V_{11} + V_{22})$$

$$(\Delta\rho)^2 = (V_{11}V_{22}) / (V_{11} + V_{22}).$$

This is the (diagonal) weighted average and its variance (as should be!).



## Off-Diagonal Weighted Average: Case Studies

$$\rho = [(V_{22} - V_{12})y_1 + (V_{11} - V_{12})y_2] / (V_{11} + V_{22} - 2V_{12})$$

### Case 1. Average of the same experimental data point

$$y_1 = y_2$$

$$\Delta y_1 = \Delta y_2 \text{ (i.e., } V_{11} = V_{22}\text{)}$$

$$c_{12} = V_{12} / (V_{11} V_{22})^{1/2} = 1 \text{ (fully correlated – same experiment)}$$

$$\rightarrow V_{11} = V_{22} = V_{12}$$

This makes the covariance matrix  $V$  singular ( $|V| = V_{11} + V_{22} - 2V_{12} = 0$ ).



## Off-Diagonal Weighted Average: Case Studies

$$p = [(V_{22} - V_{12})y_1 + (V_{11} - V_{12})y_2] / (V_{11} + V_{22} - 2V_{12})$$

$$(\Delta p)^2 = [V_{11}V_{22} - (V_{12})^2] / (V_{11} + V_{22} - 2V_{12})$$

### Case 2. Average of two experimental points with same variance

$$\Delta y_1 = \Delta y_2 \text{ (i.e., } V_{11} = V_{22}\text{)}$$

$$p = [(V_{11} - V_{12})y_1 + (V_{11} - V_{12})y_2] / (2V_{11} - 2V_{12}) = (y_1 + y_2) / 2$$

$$(\Delta p)^2 = M_{pp} = [V_{11}^2 - (V_{12})^2] / (2V_{11} - 2V_{12}) = (V_{11} + V_{12}) / 2$$



## Off-Diagonal Weighted Average: Extreme Cases

### Case 2. Average of two experimental points with same variance

$$p = [(V_{11}-V_{12})y_1 + (V_{11}-V_{12})y_2] / (2V_{11}-2V_{12}) = (y_1+y_2)/2$$

$$(\Delta p)^2 = [V_{11}^2 - (V_{12})^2] / (2V_{11}-2V_{12}) = (V_{11}+V_{12})/2$$

#### W. Mannhart (WM11 Appendix 2):

For uncorrelated data ( $V_{12}=0$ ) the variance of the average ( $\Delta p$ ) is give by half of the common variance of both data.

For correlated data ( $V_{12} \neq 0$ ) the variance of the average ( $\Delta p$ ) remains above this value for a positive value of  $V_{12}$ .

This means a positive correlation of data lessens the uncertainty reduction of an evaluated result.

In the past this effect was sometimes responsible for **inconsistencies in evaluated data**, since the neglect of covariances gave **too strong a reduction of the evaluated final uncertainties**.



## Off-Diagonal Weighted Average: Case Studies

$$p = [(V_{22} - V_{12})y_1 + (V_{11} - V_{12})y_2] / (V_{11} + V_{22} - 2V_{12})$$

**Case 3.  $V_{11} < V_{12} < V_{22}$  (or  $V_{22} < V_{12} < V_{11}$ )**

The average  $p$  is larger or smaller than BOTH  $y_1$  and  $y_2$  (!).

**Proof:**

If we define  $a = V_{22} - V_{12}$  ( $>0$ ) and  $b = V_{12} - V_{11}$  ( $>0$ ),  $p = (ay_1 - by_2) / (a - b)$ .

$$\begin{aligned}(p - y_1)(p - y_2) &= [(ay_1 - by_2) / (a - b) - y_1] \cdot [(ay_1 - by_2) / (a - b) - y_2] \\ &= ab(y_1 - y_2)^2 / (a - b) \\ &> 0\end{aligned}$$

Therefore both  $p - y_1$  and  $p - y_2$  are positive or negative.



# Generalized Least Squares

In conventional least squares, we assumed that

- covariance matrix  $\mathbf{V}$  for experimental data  $\mathbf{y}$  is diagonal.
- no variance-covariance for old model parameters  $\mathbf{p}$ .

→

Generalized least squares approach considers

- correlation in experimental data (i.e. off-diagonal elements of  $\mathbf{V}$ )
- covariance of old fitting parameters  $\mathbf{p}$

Let us see the answer of this problem *without proves!*





# Conventional v.s. General: Minimum Conditions

## Conventional least squares

$$\chi^2 = [\mathbf{y} - \mathbf{f}(\mathbf{p})]^t \mathbf{V}^{-1} [\mathbf{y} - \mathbf{f}(\mathbf{p})] = \min$$

New model parameter  $\mathbf{p}$  should be consistent with experimental data  $\mathbf{y}$  through the model  $\mathbf{f}$

## Generalized least squares

$$\chi^2 = [\mathbf{y} - \mathbf{f}(\mathbf{p})]^t \mathbf{V}^{-1} [\mathbf{y} - \mathbf{f}(\mathbf{p})] + [\mathbf{p} - \mathbf{p}_0]^t \mathbf{M}_0^{-1} [\mathbf{p} - \mathbf{p}_0] = \min$$

New model parameters  $\mathbf{p}$  should be consistent with experimental data  $\mathbf{y}$ , through the model  $\mathbf{f}$ , *and* should be consistent with old model parameters  $\mathbf{p}_0$ .



## Formulae of Generalized Least-Squares

- **Problem:**

Update model parameters  $\mathbf{p}_0 = \{p_{0j}\}$  (covariance  $\mathbf{M}_0$ ) to  $\mathbf{p} = \{p_j\}$  by experimental points  $\mathbf{y} = \{y_i\}$  (covariances  $\mathbf{V}$ ) ( $i=1, n$ ).

- Model  $\mathbf{y} \sim f(\mathbf{p})$  can be expanded around prior model parameters  $\mathbf{p}_0$  as

$$f(\mathbf{p}) \sim f(\mathbf{p}_0) + \mathbf{G}(\mathbf{y} - \mathbf{y}_0), \quad \mathbf{G} = \left. \frac{\partial f(\mathbf{p})}{\partial \mathbf{p}} \right|_{\mathbf{p}=\mathbf{p}_0} = \mathbf{G}.$$

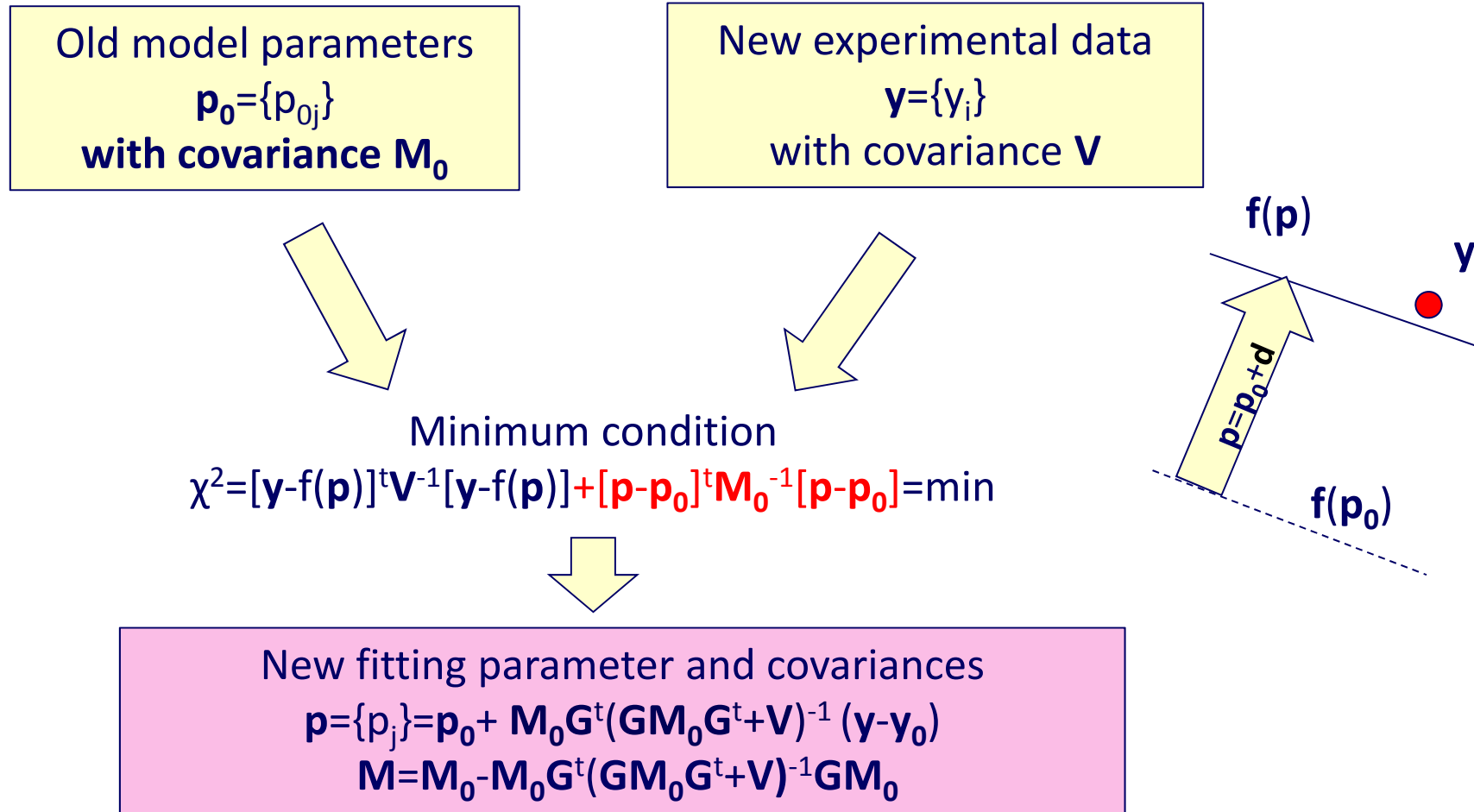
- Updated model parameters  $\mathbf{p}$  and their covariance  $\mathbf{M}$  are

$$\mathbf{p} = \mathbf{p}_0 + \mathbf{M}_0 \mathbf{G}^t (\mathbf{G} \mathbf{M}_0 \mathbf{G}^t + \mathbf{V})^{-1} (\mathbf{y} - \mathbf{y}_0)$$

$$\mathbf{M} = \mathbf{M}_0 - \mathbf{M}_0 \mathbf{G}^t (\mathbf{G} \mathbf{M}_0 \mathbf{G}^t + \mathbf{V})^{-1} \mathbf{G} \mathbf{M}_0$$



# Flow of Generalized Least-Squares



## Summary

### Generalized least-squares:

Prior model parameters  $\mathbf{p}_0$  (covariance  $\mathbf{M}_0$ ) are updated by experimental data  $\mathbf{y}$  (covariance  $\mathbf{V}$ ) by

$$\mathbf{p} = \mathbf{p}_0 + \mathbf{M}_0 \mathbf{G}^t (\mathbf{G} \mathbf{M}_0 \mathbf{G}^t + \mathbf{V})^{-1} (\mathbf{y} - \mathbf{y}_0)$$
$$\mathbf{M} = \mathbf{M}_0 - \mathbf{M}_0 \mathbf{G}^t (\mathbf{G} \mathbf{M}_0 \mathbf{G}^t + \mathbf{V})^{-1} \mathbf{G} \mathbf{M}_0$$

### Weighted average:

The weighted average of two data  $y_1$  and  $y_2$  and its variance are

$$p = [(V_{22} - V_{12})y_1 + (V_{11} - V_{12})y_2] / (V_{11} + V_{22} - 2V_{12})$$
$$(\Delta p)^2 = [V_{11}V_{22} - (V_{12})^2] / (V_{11} + V_{22} - 2V_{12})$$

The off-diagonal element  $V_{12}$  (i.e., correlation) plays an important role.



## Exercise (~13:00)

Choose the following tasks as you like:

- Paper 2.2 (Weighted average with and without covariance)
- Paper 2.3 (Preparation of input for least-squares analysis)
- Paper 2.4 (Weighted average with covariance).
- Go for lunch.

