



Metti⁵

Lecture L2 : Basics for linear inversion, the 'white box' case

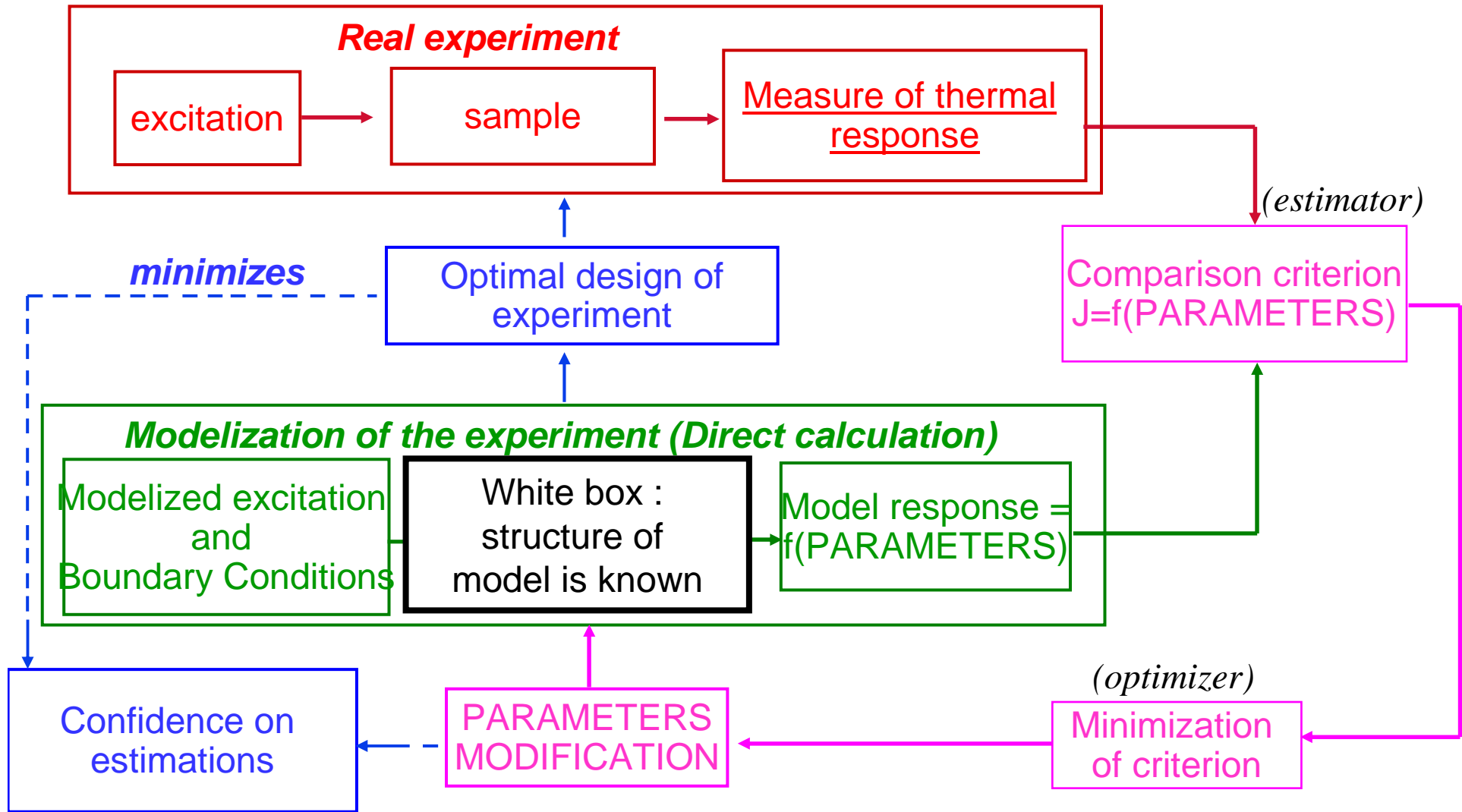
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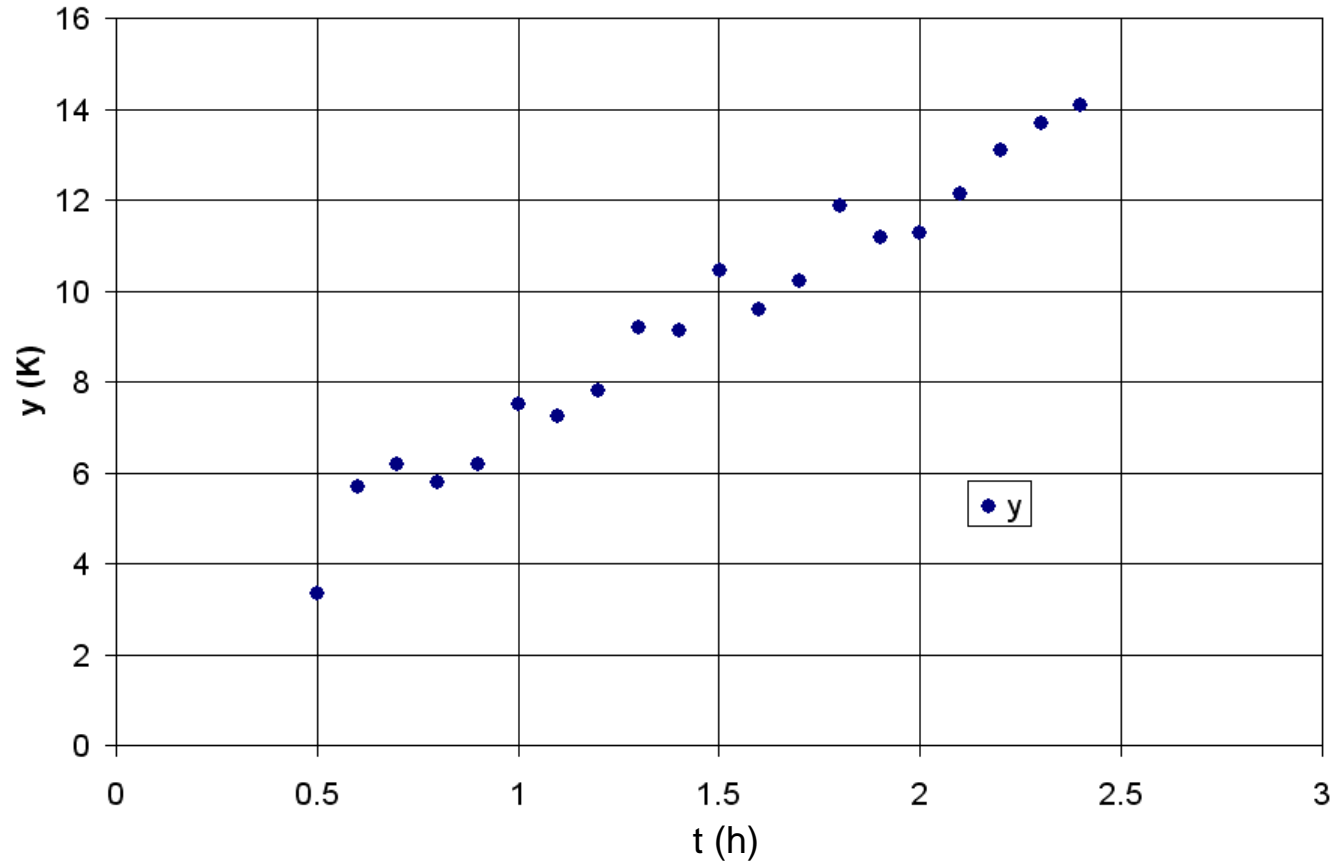
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General context, white box case



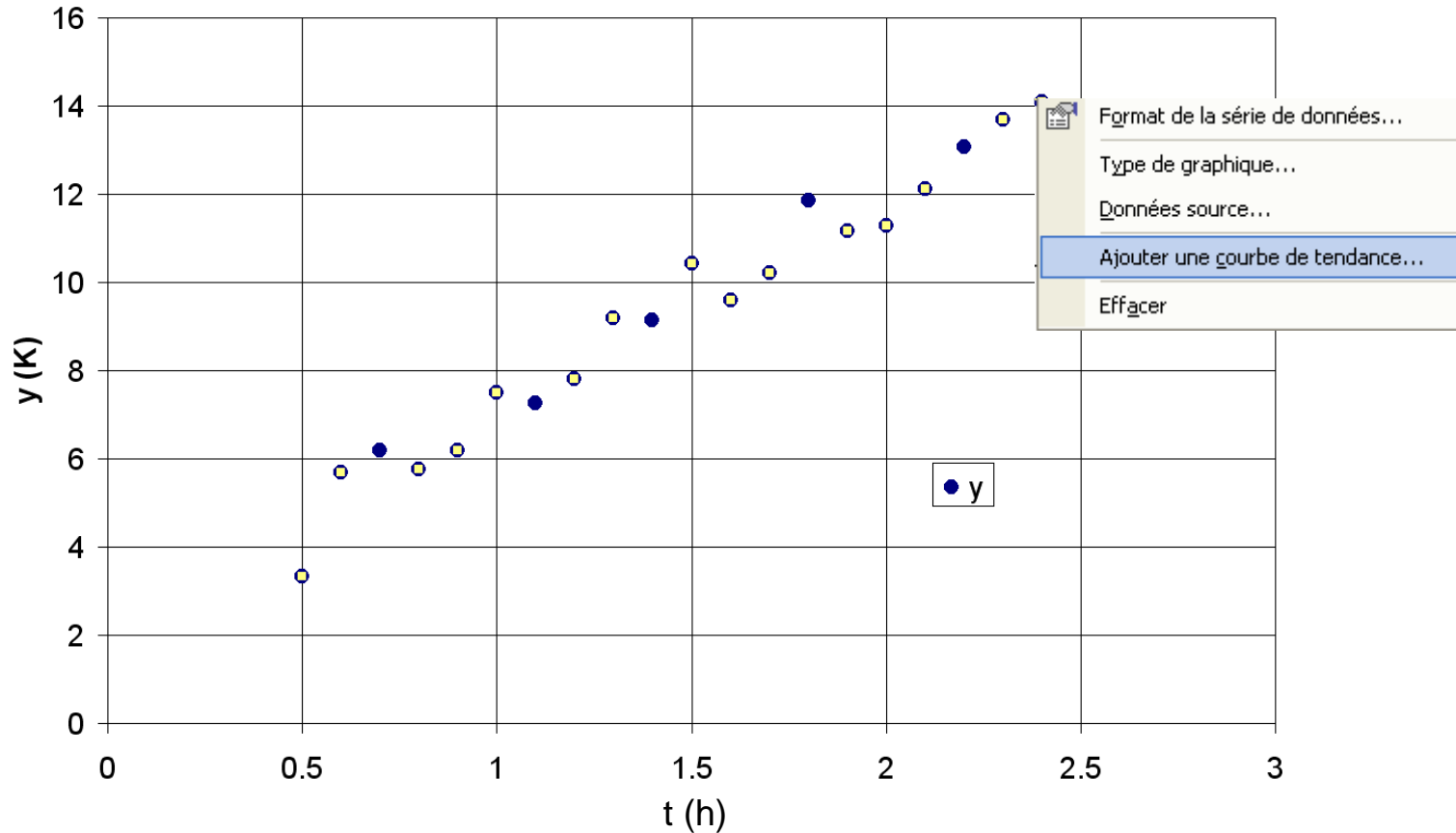
First : Beyond the magic of 'trendline tool' (‘courbe de tendance’ in français...)

20 measurements y_i at 20 times t_i , $i=1$ to 20



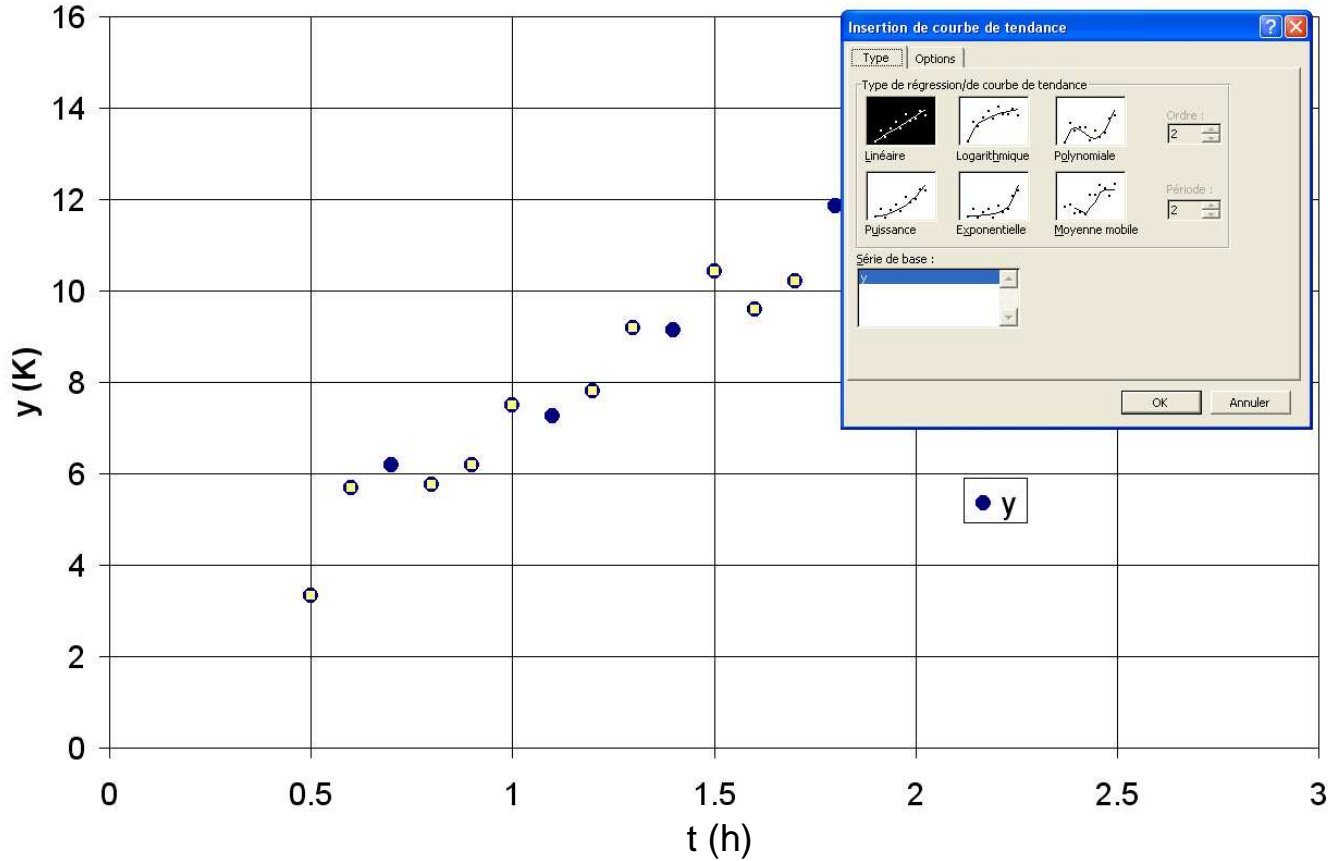
Beyond the magic of 'trendline tool'

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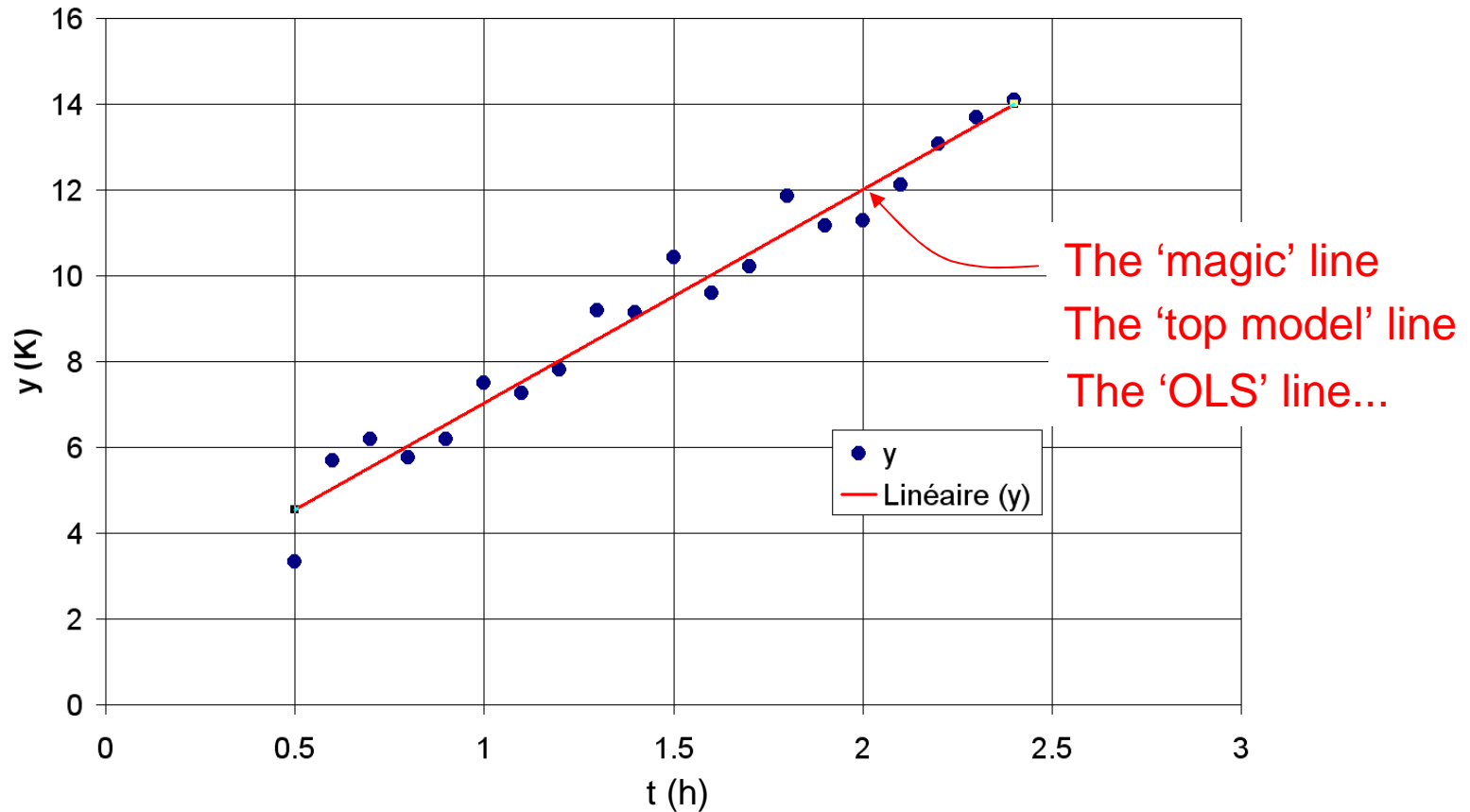
Beyond the magic of 'trendline tool'

20 measurements y_i at 20 times t_i , $i=1$ to 20



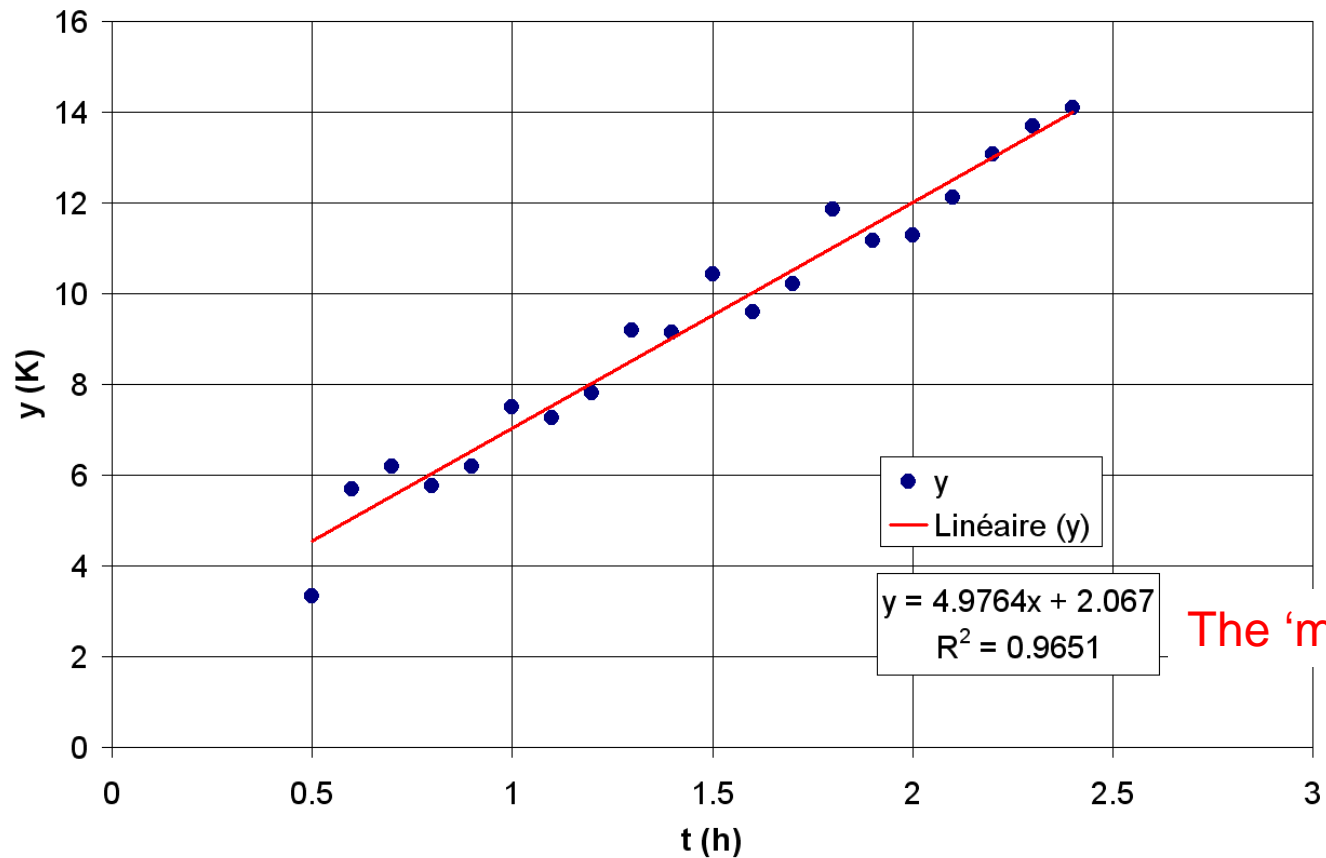
Beyond the magic of 'trendline tool'

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Beyond the magic of 'trendline tool'

20 measurements y_i at 20 times t_i , $i=1$ to 20

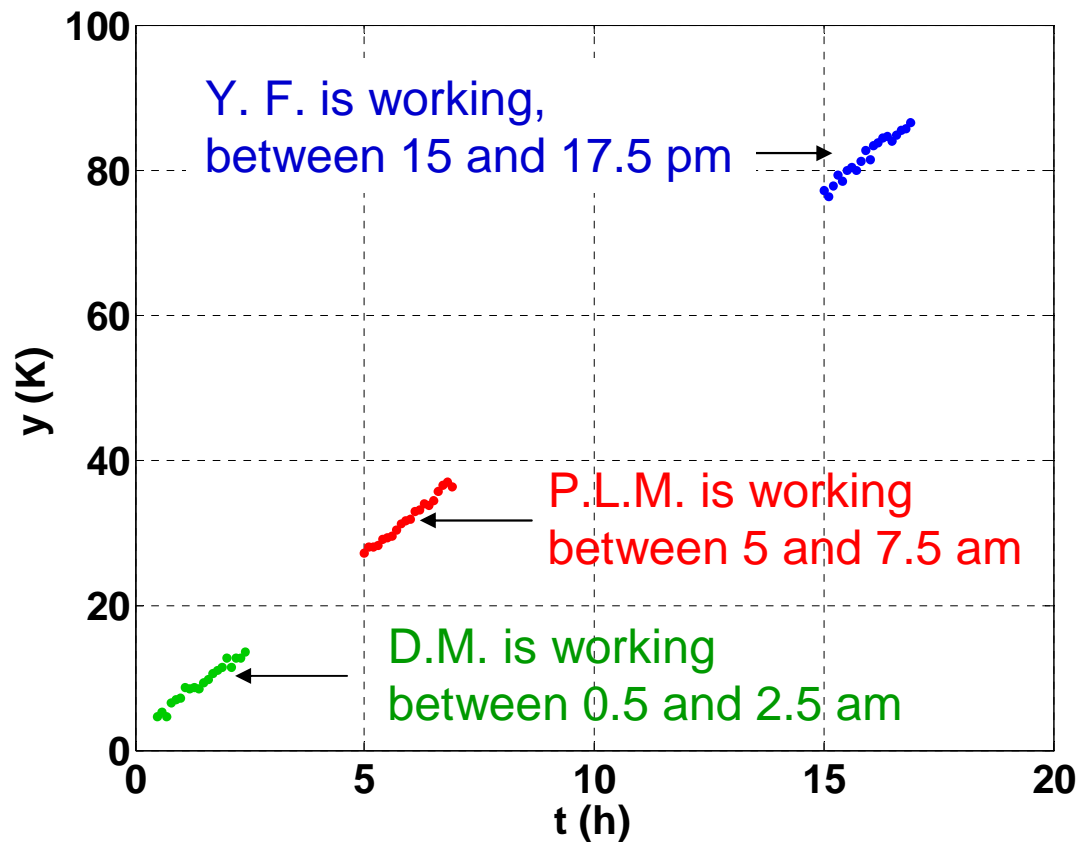


The 'magic' model

Let's play with the trendline tool, and let's observe what happens...

Let's play with the 'trendline tool'

A researcher (names Y. J.) works with three students, on an experiment that begins at 0.00 o'clock and that is during about 20h. Each student performs $m=20$ measurements y_i . Each measurement is done with the same accuracy.



Y. J. suspects that every measurement can be explained by the simple model :

$$y_{mo} = x_1 t + x_2$$

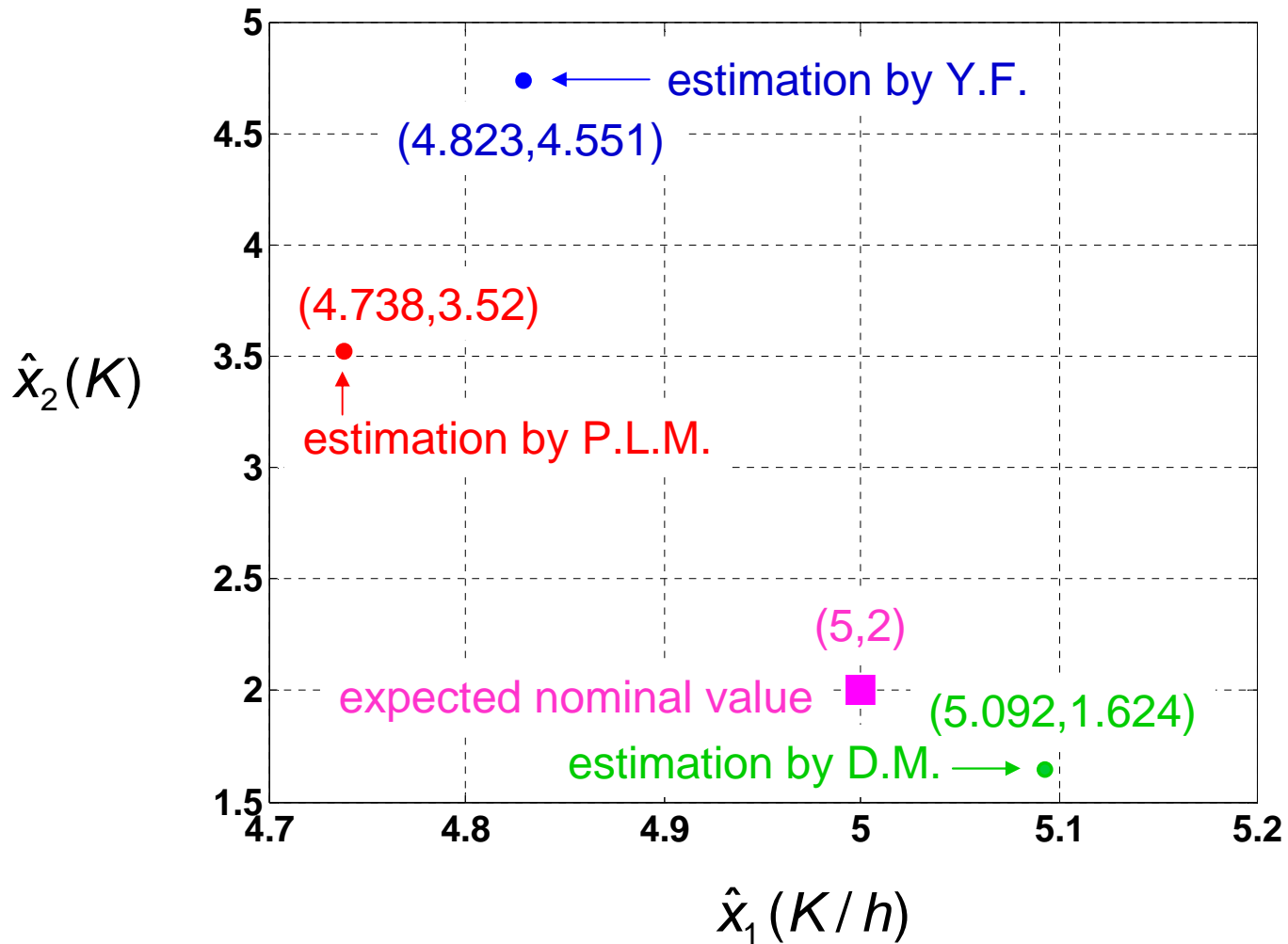
He also expects the values

$$x_1 = x_1^{nom} = 5 \text{ K/h}$$

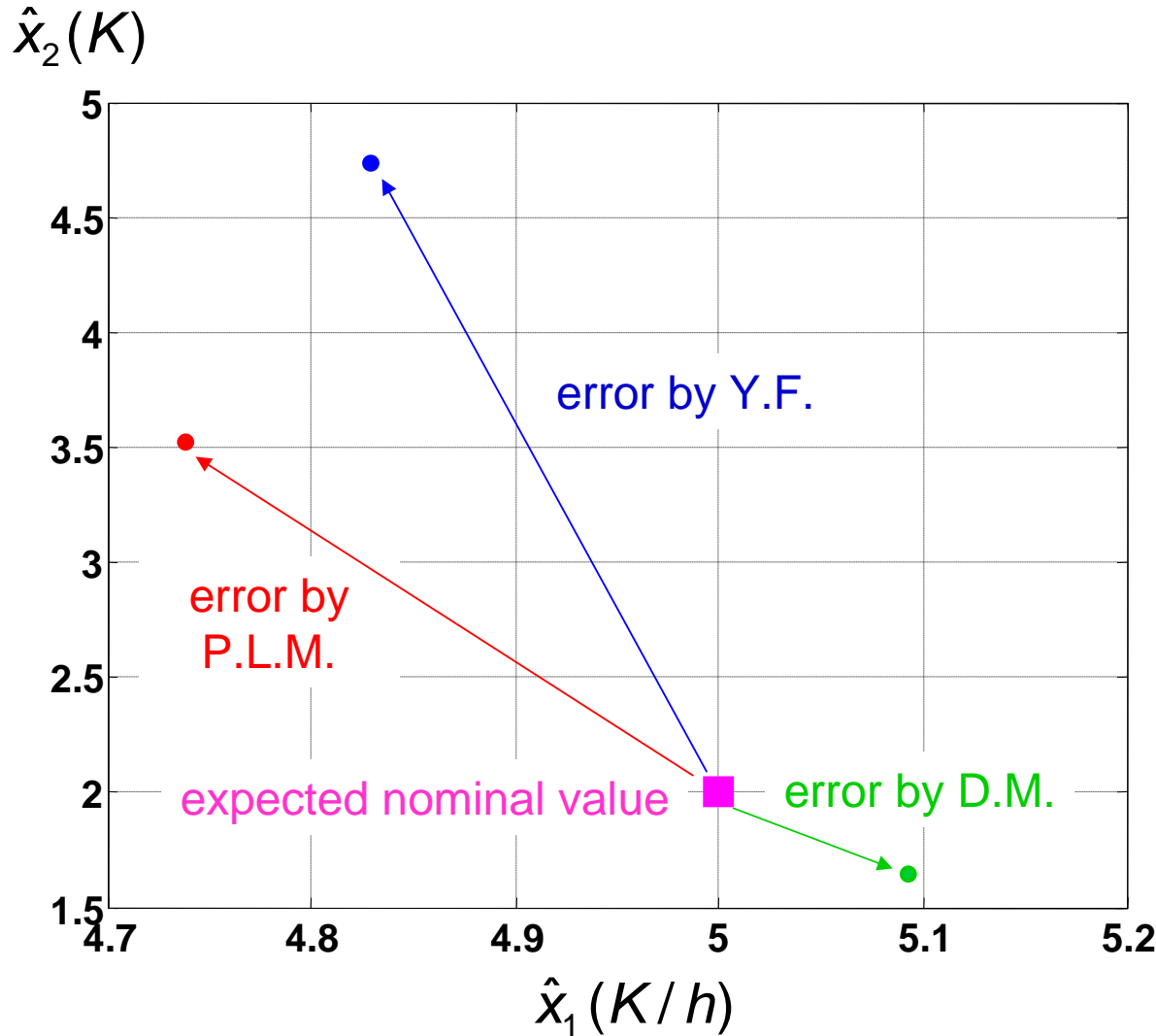
$$x_2 = x_2^{nom} = 2 \text{ K}$$

...but keep them secret... He asks each student to use the trendline tool on his own 20 measurements and give him the value of x_1 and x_2

Result of estimations in the 'estimation plane'



Result of estimations in the 'estimation plane'



- each student gives a different result
- each student is at a different distance from the expected value

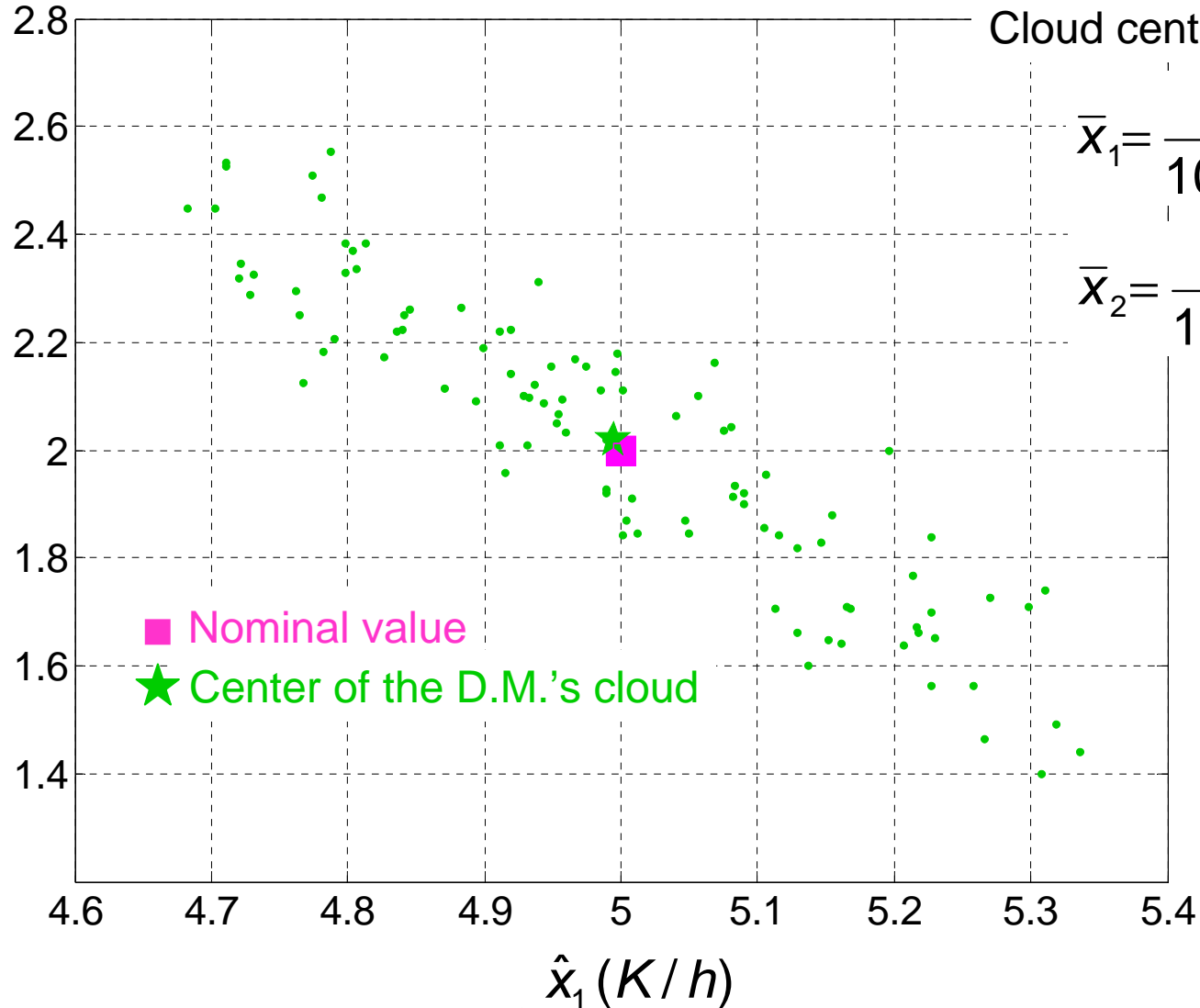


One way to be sure :
 « Do experiment and parameter estimation again! And again, and again.... ! »

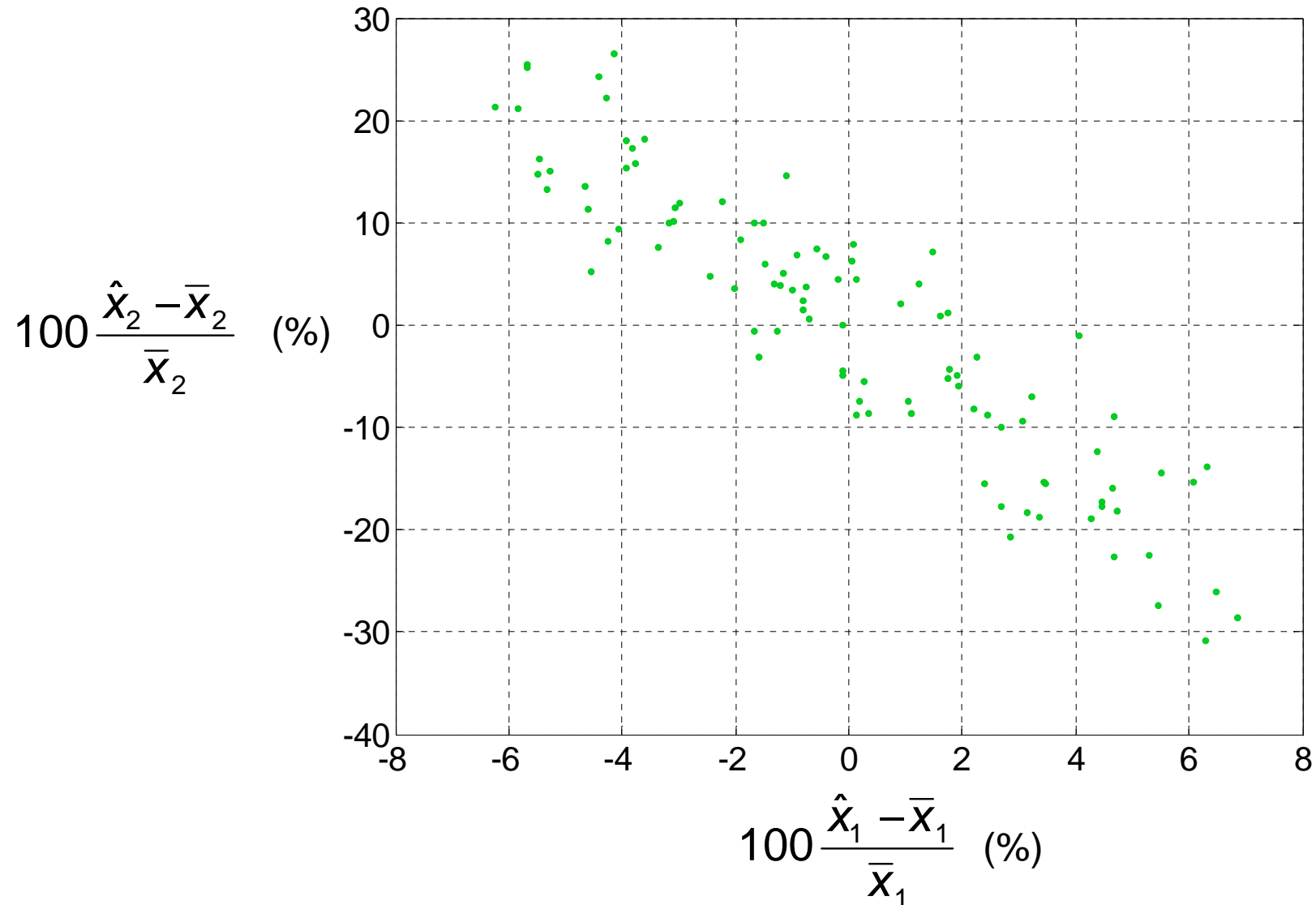
The experiment is the same...
 excepted the random part of it :
 the noise measurement

Cloud of 100 estimations $(\hat{x}_{1,i}, \hat{x}_{2,i})$ for D.M.

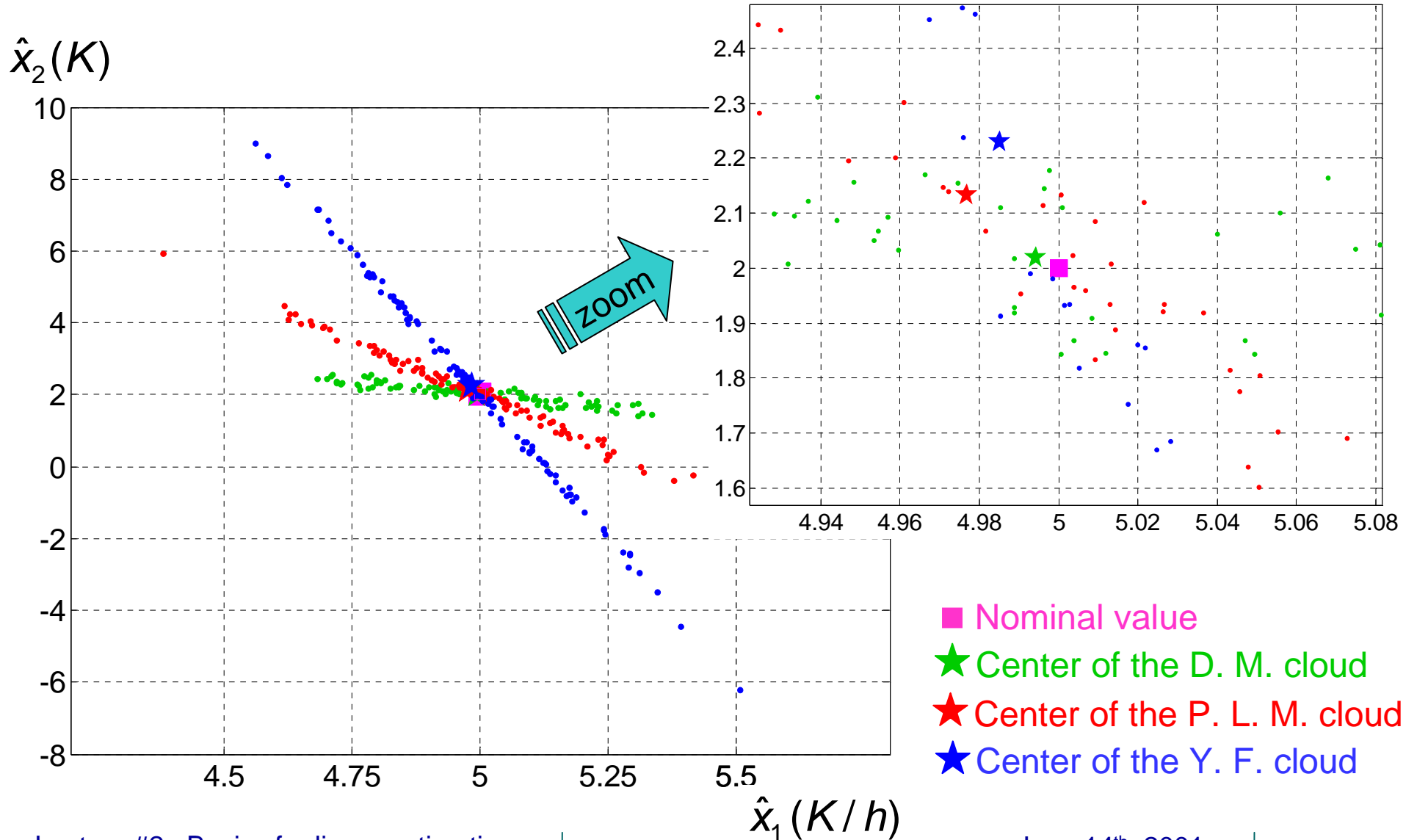
$\hat{x}_2(K)$



Relative scattering of D.M.'s cloud around its center



Three clouds of 100 estimations $(\hat{x}_{1,i}, \hat{x}_{2,i})$



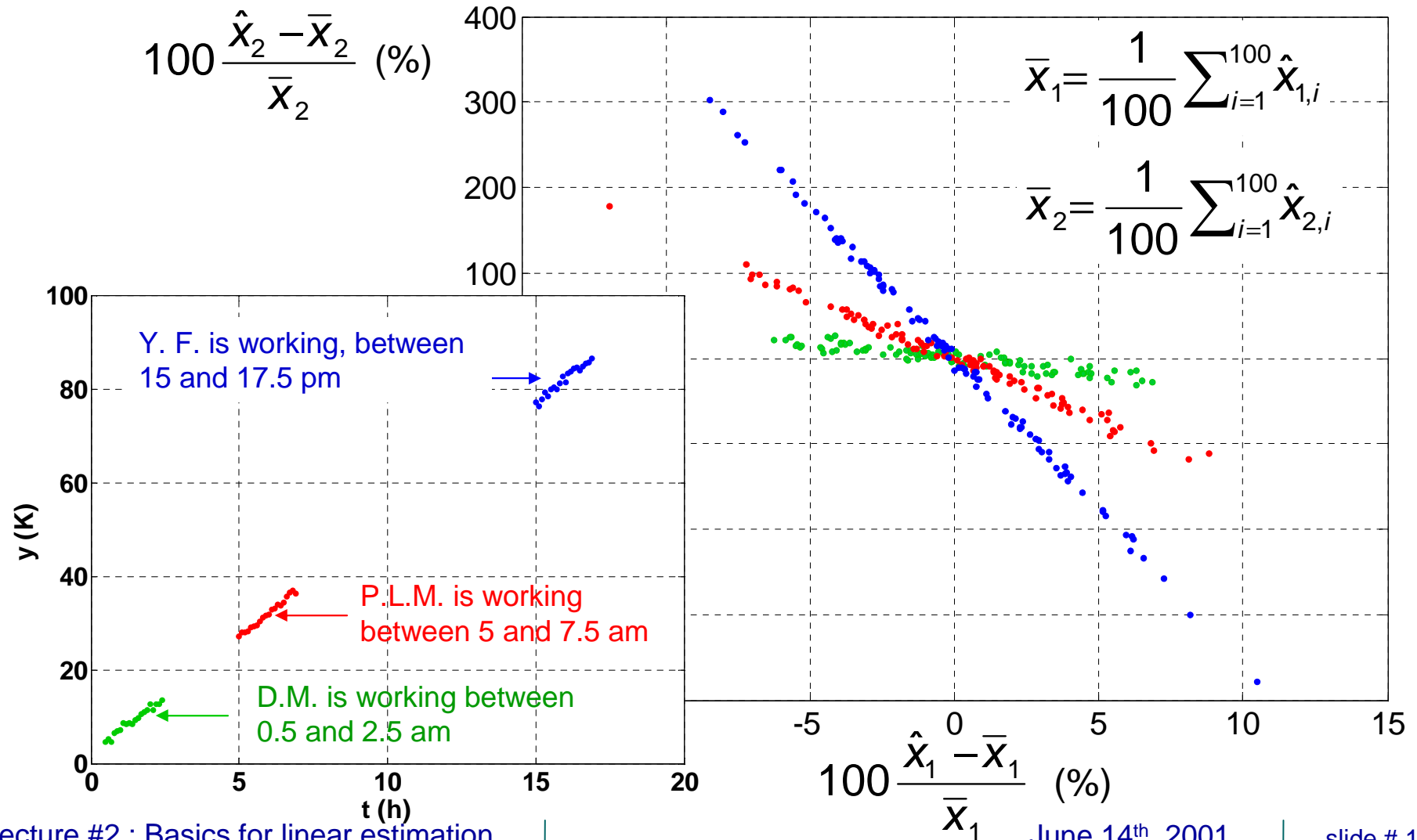
Relative scattering of each cloud around its center

Cloud center coordinates :

$$100 \frac{\hat{X}_2 - \bar{X}_2}{\bar{X}_2} (\%)$$

$$\bar{X}_1 = \frac{1}{100} \sum_{i=1}^{100} \hat{x}_{1,i}$$

$$\bar{X}_2 = \frac{1}{100} \sum_{i=1}^{100} \hat{x}_{2,i}$$



Each student can announce now :

- the central value of its cloud of 100 estimations
- a size of the region (absolute and relative) in which are located the majority of its estimations

Student	D.M.	P.L.M.	Y.F.
Time range (h)	0.5 h -2.5 h	5 h -7.5 h	15 h -17.5 h
Central value \bar{X}_1 (K/h)	4.994 K/h	4.738 K/h	4.985 K/h
Absolute interval (K/h)	± 0.3 K/h	± 0.35 K/h	± 0.35 K/h
Relative interval (%)	± 6 %	± 7 %	± 7 %
Central value \bar{X}_2 (K)	2.019	3.52	2.223
Absolute interval (K)	± 0.5 K	± 1 K/h	± 5.3 K/h
Relative interval (%)	± 10 %	± 28 %	± 106 %

- Finally we can say that to the question :

‘Find the x_1 and x_2 values of model $y_{mo} = x_1 t + x_2$,
 given m measurements y_i at t_i ’

the answer is not :

‘a unique point (\hat{x}_1, \hat{x}_2) ’

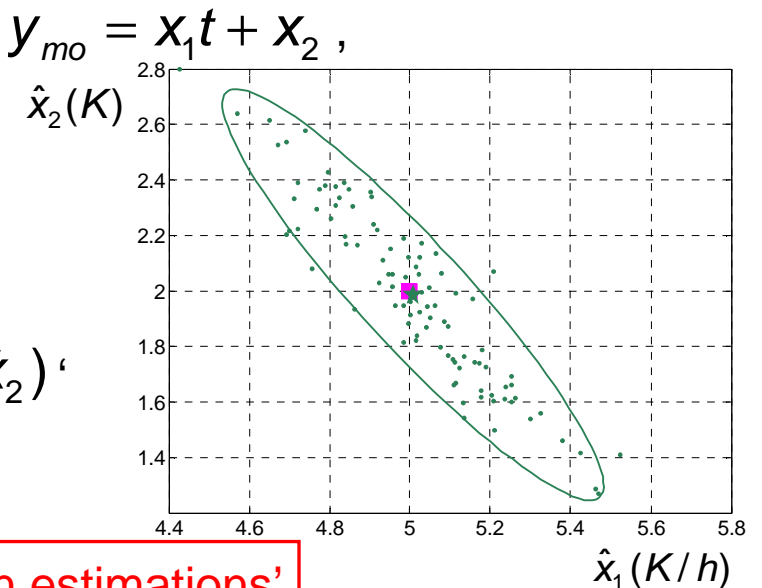
but rather :

‘a SPOT (or a cloud) of points (\hat{x}_1, \hat{x}_2) ’

because of random noise measurement.

In other words :

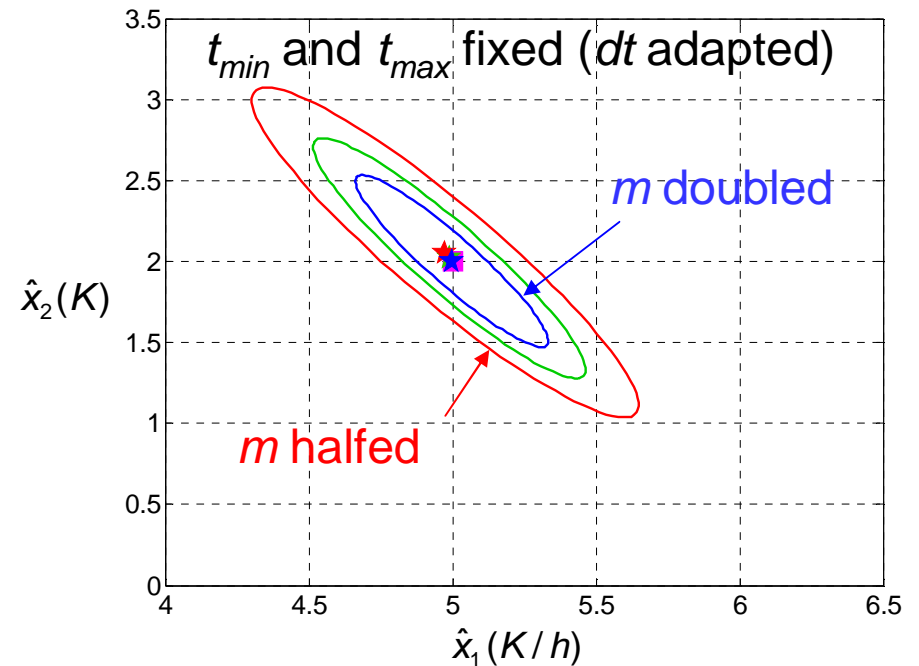
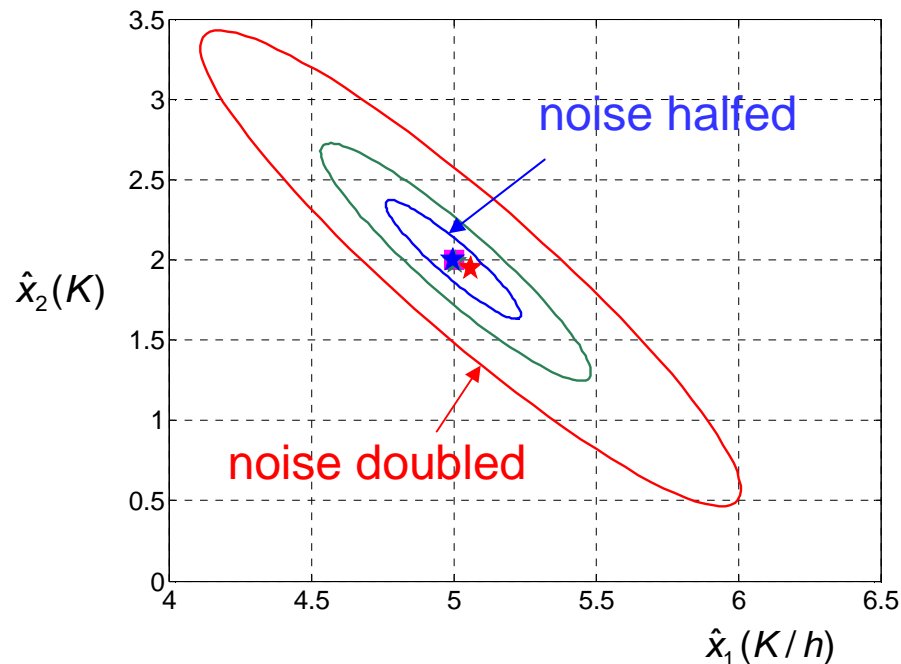
‘Blur on measurements gives blur on estimations’



- Here clouds of estimations have elliptical shapes with high density in the central region
- The center of each spot is very close to the nominal value
- The **ideal spot** would be : - with the ‘smallest’ extension
 - **centered on the nominal value**

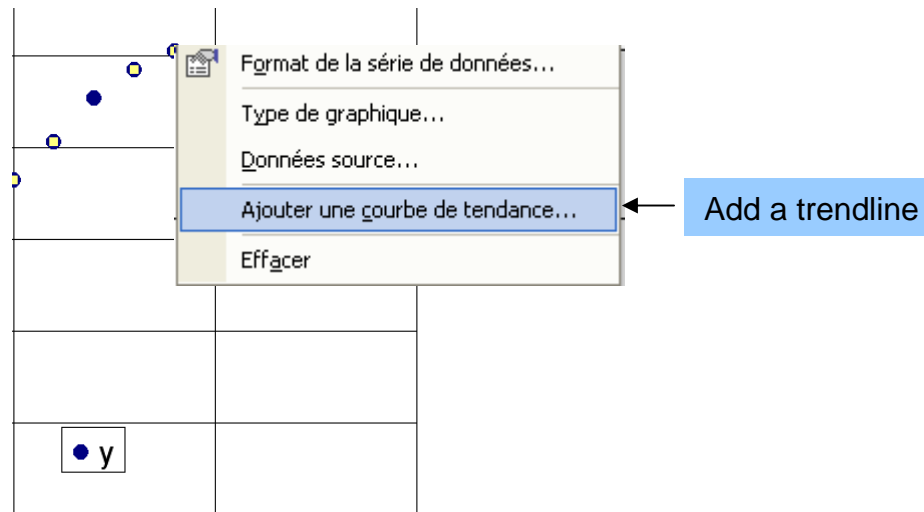
Next comments : influence of experimental conditions

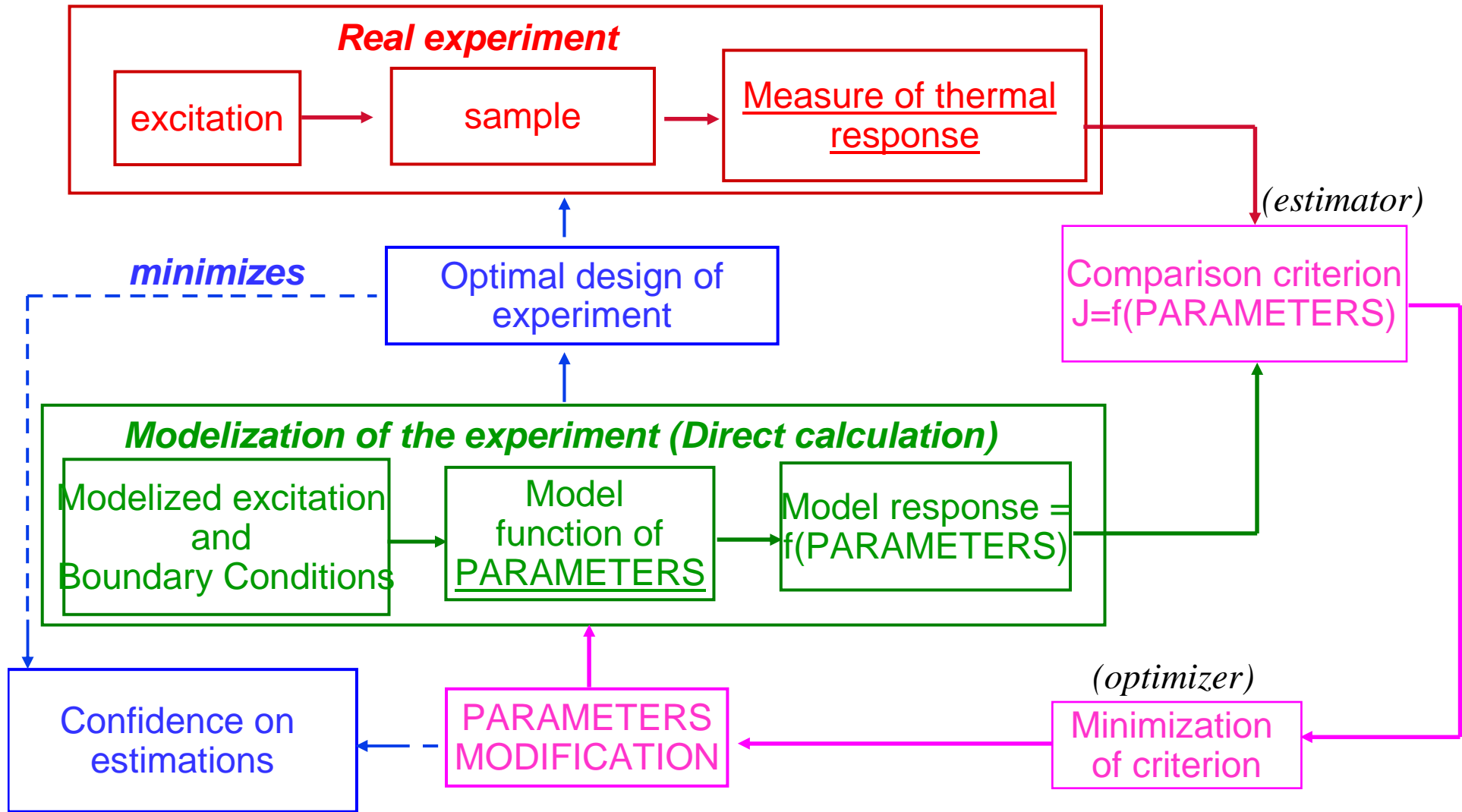
- It seems that certain experimental conditions are better than others :
 - here, measurements have to be 'close' to $t=0$
- Suppose we know the equation of the elliptical solution spot (detailed later) :
 - What happens if noise measurement magnitude changes ?
 - What happens if number of measurements ($m=20$) changes ?

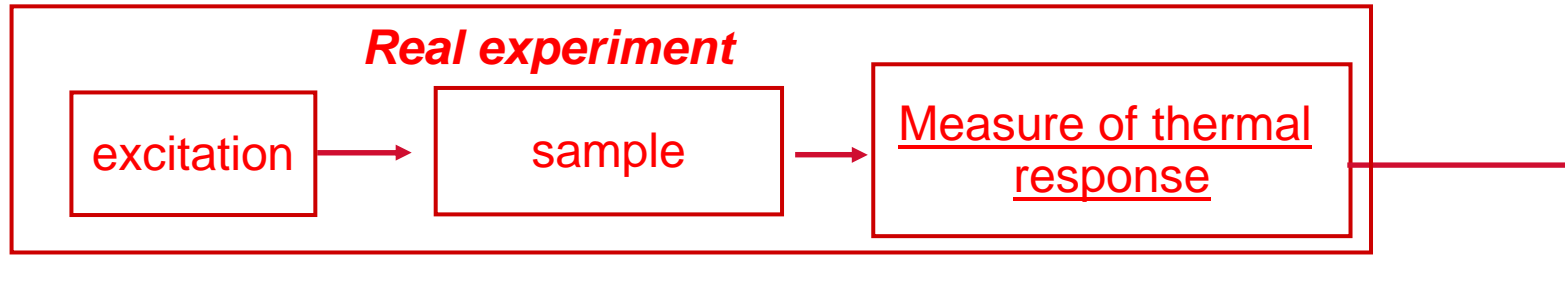


Back to the magic...

- So it would be very interesting to predict the performances of a parameter estimation method in term of 'spot (or cloud) of estimations' **without achieving 100 experiment/identifications!**
- We must try to predict the shape of the 'spot of estimations' (that will be called 'the confidence region'), associated to only one **experiment/identification realisation**
- But before, we have to reveal the secret of the '**magic/top model/OLS line**'...







$(m \times 1)$ experimental measurements vector

$$\mathbf{y} = [y_1 \dots y_i \dots y_m]^t \quad \text{with} \quad y_i = y(t_i), \quad t_i = t_{\min} + (i-1).dt, \quad i=1, \dots, m$$

$(m \times 1)$ time vector (explicative variable)

$$\mathbf{t} = [t_1 \dots t_i \dots t_m]^t$$

y_i

$(m \times 1)$ measurement errors vector

$$\boldsymbol{\varepsilon} = [\varepsilon_1 \dots \varepsilon_i \dots \varepsilon_m]^t \quad \varepsilon_i \quad \text{be the (unknown) error associated to the measurement}$$

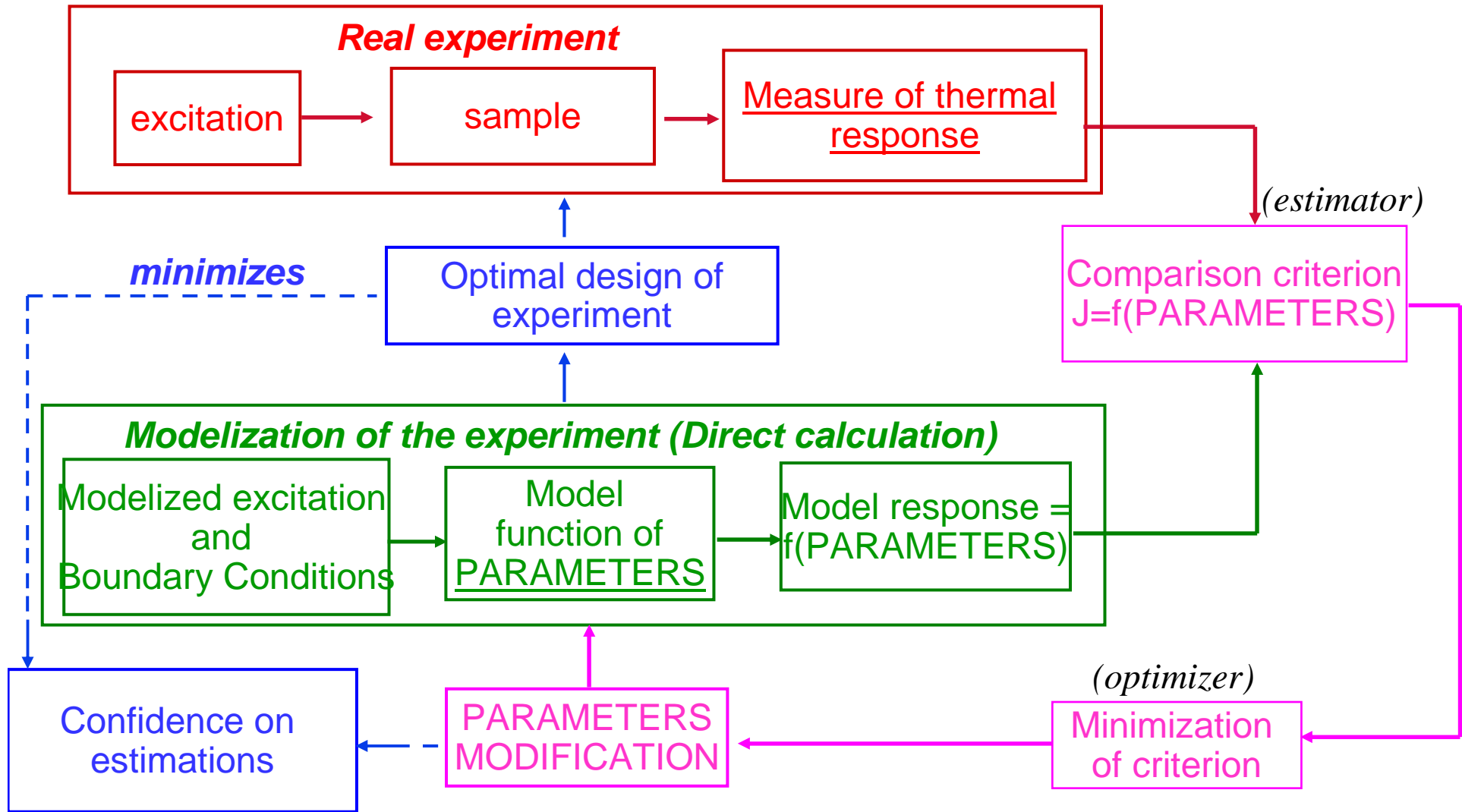
Some assumptions have to be done on these measurement errors.

Number	Assumption on measurement errors	Explanation
1	Additive errors	$\mathbf{y} = \mathbf{y}_{perfect} + \boldsymbol{\varepsilon}$
2	Unbiased model	$\mathbf{y}_{perfect} = \mathbf{y}_{mo}(\mathbf{x}^{exact})$
3	Zero mean errors	$E[\boldsymbol{\varepsilon}] = 0$
4	Constant variance	$Var[\boldsymbol{\varepsilon}] = \sigma_{\varepsilon}^2$
5	Uncorrelated errors	$Cov[\varepsilon_i, \varepsilon_j] = 0$ for $i \neq j$
6	Normal probability distribution	
7	Known statistical parameters	
8	No error in the X_{ij}	\mathbf{X} is not a random matrix
9	No prior information regarding the parameters	

$E[.]$ Is the expected value operator (representing the mean of a large number of realizations of the random variable)

Covariance Matrix of measurement errors

$$\boldsymbol{\Psi} = E[(\boldsymbol{\varepsilon} - E[\boldsymbol{\varepsilon}])(\boldsymbol{\varepsilon} - E[\boldsymbol{\varepsilon}])^t] = E[\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^t] = \text{diag}(\sigma_{\varepsilon}^2, \dots, \sigma_{\varepsilon}^2, \dots, \sigma_{\varepsilon}^2) = \mathbf{I} \cdot \sigma_{\varepsilon}^2$$

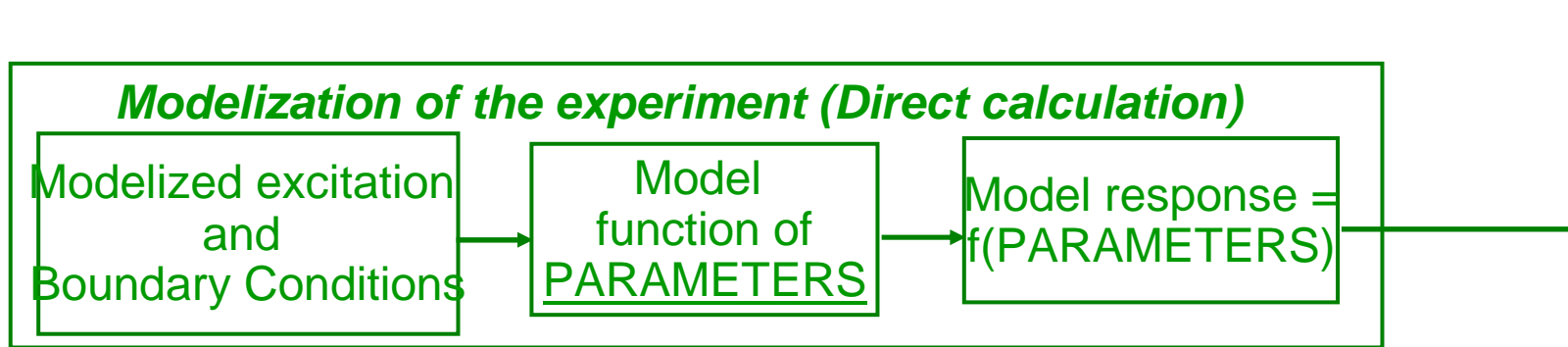


$(m \times 1)$ experimental measurements vector

$$\mathbf{y}_{mo}(\mathbf{t}, \mathbf{x}) = [y_{mo,1}(t_1, \mathbf{x}) \dots y_{mo,i}(t_i, \mathbf{x}) \dots y_{mo,m}(t_m, \mathbf{x})]^t$$

with $y_{mo}(t, \mathbf{x}) = \eta(t, \mathbf{x})$

parameters vector $(n \times 1)$: $\mathbf{x} = [x_1 \dots x_n]^t$



With here: $y_{mo}(t, \mathbf{x}) = x_1 t + x_2$

$$y_{mo}(t, \mathbf{x}) = x_1 t + x_2$$

NB : that model is said 'linear' on the parameter estimation point of view because it is linear with respect to its parameter x_i . The following model

$$y_{mo}(t, \mathbf{x}) = x_1 \sqrt{t} + x_2 \cdot \text{erf}(t)$$

is still linear with respect to its parameter x_i even it is not with respect to time. The following model

$$y_{mo}(t, \mathbf{x}) = x_1 \sqrt{t} + \exp(-x_2 t)$$

is not linear with respect to x_2

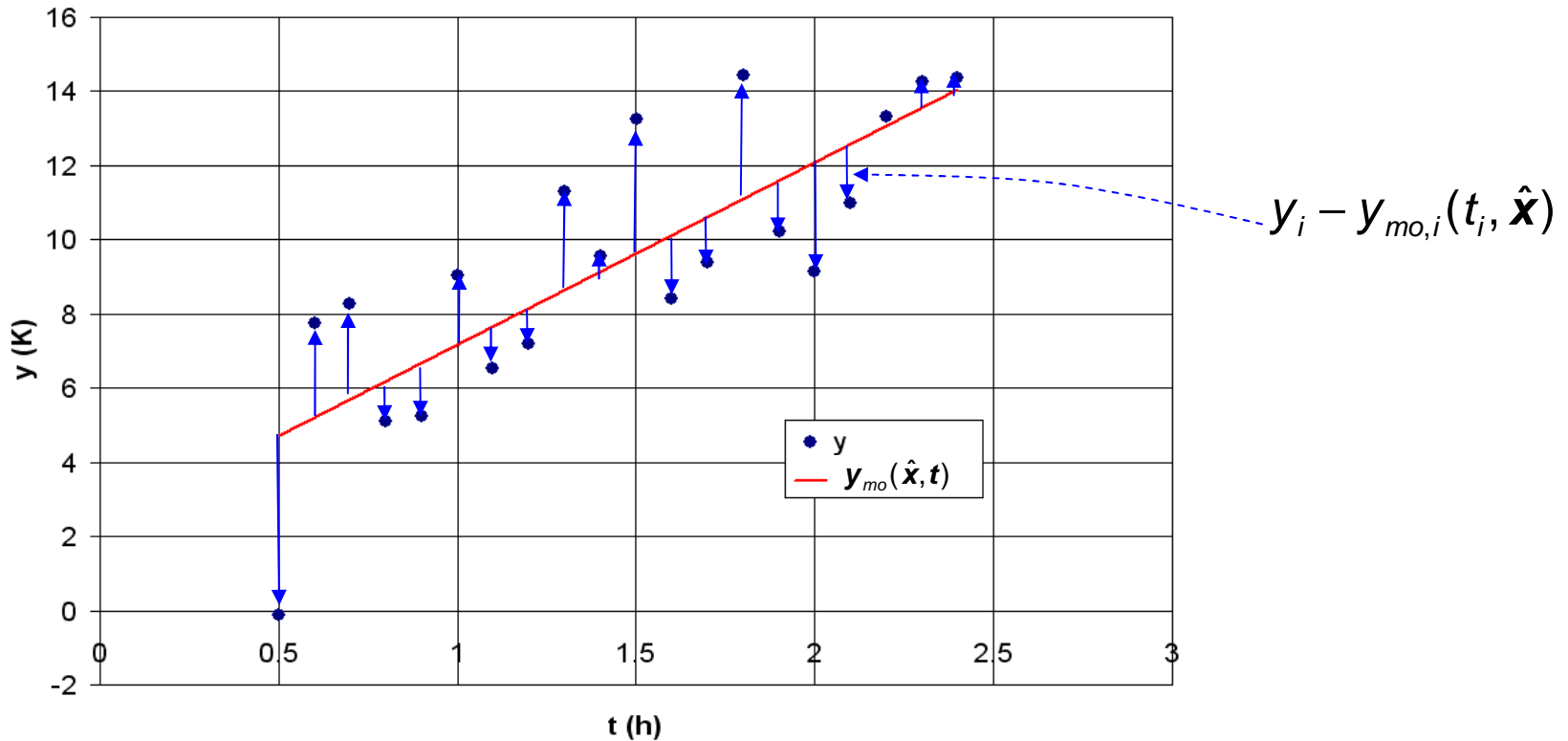
Writing the m model values for the m time values, the m resulting equations can be written in a matrix way as following :

$$\begin{bmatrix} y_{mo,1} \\ \vdots \\ y_{mo,i} \\ \vdots \\ y_{mo,m} \end{bmatrix} = \begin{bmatrix} t_1 & 1 \\ \vdots & \vdots \\ t_i & 1 \\ \vdots & \vdots \\ t_m & 1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \text{or} \quad \boxed{y_{mo} = \mathbf{S}\mathbf{x}} \quad \text{with} \quad \mathbf{S} = \begin{bmatrix} S_1(t_1) & S_2(t_1) \\ \vdots & \vdots \\ S_1(t_i) & S_2(t_1) \\ \vdots & \vdots \\ S_1(t_m) & S_2(t_1) \end{bmatrix} = \begin{bmatrix} t_1 & 1 \\ \vdots & \vdots \\ t_i & 1 \\ \vdots & \vdots \\ t_m & 1 \end{bmatrix}$$

Sensitivity matrix

with $S_k(t, \mathbf{x}) = \left. \frac{\partial y_{mo}(t, \mathbf{x})}{\partial x_k} \right|_{t, x_j \text{ for } j \neq k}$: sensitivity coefficient relative to parameter $x_k, k=1, \dots, n$

Problem : use the $m(=20)$ measurements to estimate the n (2) unknown parameters :
Overdetermined problem transformed in a minimization problem :



Residual vector ($m \times 1$)

$$\mathbf{r}(\hat{\mathbf{x}}) = \mathbf{y} - \mathbf{y}_{mo}(\hat{\mathbf{x}}) = [y_1 - y_{mo,1}(t_1, \hat{\mathbf{x}}) \quad \dots \quad y_i - y_{mo,i}(t_i, \hat{\mathbf{x}}) \quad \dots \quad y_m - y_{mo,m}(t_m, \hat{\mathbf{x}})]^t$$

Without any a priori information on the parameters and given the above assumptions for measurements errors, the square of the Euclidian norm of the residual vector is minimised :

$$J_{OLS}(\hat{\mathbf{x}}) = \|\mathbf{r}(\hat{\mathbf{x}})\|^2 = \|\mathbf{y} - \mathbf{S}\hat{\mathbf{x}}\|^2$$

This scalar number is called the Ordinary Least Squares (OLS) cost function

$$J_{OLS}(\hat{\mathbf{x}}) = \sum_{i=1}^m r_i(\hat{\mathbf{x}})^2 = \sum_{i=1}^m \left(y_i - \sum_{j=1}^n S_j(t_i)\hat{x}_j \right)^2 = \sum_{i=1}^m (y_i - y_{mo,i}(t_i, \hat{\mathbf{x}}))^2$$

With a matrix formulation it gives :

$$J_{OLS}(\hat{\mathbf{x}}) = [\mathbf{y} - \mathbf{y}_{mo}(\hat{\mathbf{x}})]^t [\mathbf{y} - \mathbf{y}_{mo}(\hat{\mathbf{x}})]$$

$$J_{OLS}(\hat{\mathbf{x}}) = [\mathbf{y} - \mathbf{S}\hat{\mathbf{x}}]^t [\mathbf{y} - \mathbf{S}\hat{\mathbf{x}}]$$

The solution of the problem is then : $\hat{\mathbf{x}}_{OLS} = \arg[\min(J_{OLS}(\hat{\mathbf{x}}))]$

The OLS estimator is the one that minimizes the scalar function $J_{OLS}(\hat{\mathbf{x}})$

$$\nabla_{\mathbf{x}} J_{OLS}(\hat{\mathbf{x}}_{OLS}) = 0 \quad \text{with} \quad \nabla_{\mathbf{x}} = \begin{pmatrix} \frac{\partial}{\partial x_1} \\ \vdots \\ \frac{\partial}{\partial x_n} \end{pmatrix}$$

$$\nabla_{\mathbf{x}} J_{OLS}(\hat{\mathbf{x}}) = 2[\nabla_{\mathbf{x}}[\mathbf{y} - \mathbf{y}_{mo}(\hat{\mathbf{x}})]]^t [\mathbf{y} - \mathbf{y}_{mo}(\hat{\mathbf{x}})]$$

Knowing that $\mathbf{S}^t = [\nabla_{\mathbf{x}} \mathbf{y}_{mo}(\hat{\mathbf{x}})]^t$ and $\mathbf{y}_{mo}(\hat{\mathbf{x}}) = \mathbf{S}\hat{\mathbf{x}}$

$$\nabla_{\mathbf{x}} J_{OLS}(\hat{\mathbf{x}}) = -2\mathbf{S}^t [\mathbf{y} - \mathbf{S}\hat{\mathbf{x}}]$$

Then $\hat{\mathbf{x}}_{OLS}$ is solution of : $[\mathbf{S}^t \mathbf{S}] \hat{\mathbf{x}}_{OLS} = \mathbf{S}^t \mathbf{y}$ (the Normal Equation)

→ $\hat{\mathbf{x}}_{OLS} = [\mathbf{S}^t \mathbf{S}]^{-1} \mathbf{S}^t \mathbf{y}$

NB : $[\mathbf{S}^t \mathbf{S}]^{-1} \mathbf{S}^t$ (nxm) is the Moore Penrose matrix

If we distinguish parameters to be estimated \mathbf{x}_r from parameters that will be fixed \mathbf{x}_c

$$\mathbf{y}_{mo}(\mathbf{x}) = \mathbf{S}\mathbf{x} = \mathbf{S}_r \mathbf{x}_r + \mathbf{S}_c \mathbf{x}_c$$

$$\mathbf{S} = [\mathbf{S}_r \vdots \mathbf{S}_c] = \begin{bmatrix} \left[\begin{array}{ccc} S_1(t_1) & \dots & S_r(t_1) \end{array} \right] & \vdots & \left[\begin{array}{ccc} S_{r+1}(t_1) & \dots & S_q(t_1) \end{array} \right] \\ \vdots & \dots & \vdots \\ \left[\begin{array}{ccc} S_1(t_m) & \dots & S_r(t_m) \end{array} \right] & \vdots & \left[\begin{array}{ccc} S_{r+1}(t_m) & \dots & S_q(t_m) \end{array} \right] \end{bmatrix}$$

→ $\hat{\mathbf{x}}_{OLS} = [\mathbf{S}_r^t \mathbf{S}_r]^{-1} \mathbf{S}_r^t (\mathbf{y} - \mathbf{S}_c \mathbf{x}_c)$

→ Matrix $\mathbf{S}^t \mathbf{S}$ needs to be inverted

$\mathbf{e}_r = \hat{\mathbf{x}}_{r,OLS}(\tilde{\mathbf{x}}_c) - \mathbf{x}_r^{exact}$: error on estimations

$\mathbf{e}_c = \tilde{\mathbf{x}}_c - \mathbf{x}_c^{exact}$: deterministic error (bias) on parameter

$\hat{\mathbf{x}}_{r,OLS}(\tilde{\mathbf{x}}_c) = \mathbf{A}_r(\mathbf{y} - \mathbf{S}_c \tilde{\mathbf{x}}_c)$ and $\mathbf{y} = \mathbf{y}_{mo}(\mathbf{x}^{exact}) + \boldsymbol{\varepsilon} = \mathbf{S}_r \mathbf{x}_r^{exact} + \mathbf{S}_c \mathbf{x}_c^{exact} + \boldsymbol{\varepsilon}$

$$\rightarrow \mathbf{e}_r = \hat{\mathbf{x}}_{r,OLS}(\tilde{\mathbf{x}}_c) - \mathbf{x}_r^{exact} = \mathbf{A}_r \boldsymbol{\varepsilon} - \mathbf{A}_r \mathbf{S}_c \mathbf{e}_c = \mathbf{e}_{r1} + \mathbf{e}_{r2}, \quad \mathbf{A}_r = [\mathbf{S}_r^t \mathbf{S}_r]^{-1} \mathbf{S}_r^t$$

Random contribution due to
random measurement
errors

the non-random (deterministic)
contribution to the total error vector
due to the deterministic error on the
fixed parameters

Covariance of estimations

$$\mathbf{C}_1 = \text{cov}(\mathbf{e}_{r1}) = E[\mathbf{e}_{r1} \mathbf{e}_{r1}^t] = \mathbf{A}_r E[\boldsymbol{\varepsilon} \boldsymbol{\varepsilon}^t] \mathbf{A}_r^t = \mathbf{A}_r \boldsymbol{\Psi} \mathbf{A}_r^t = \boxed{[\mathbf{S}_r^t \mathbf{S}_r]^{-1} \sigma_\varepsilon^2 = \mathbf{C}_1}$$

→ $[\mathbf{S}_r^t \mathbf{S}_r]^{-1}$ is a matrix ($r \times r$) that amplifies the noise measurements
(we have found the danger!)

Bias of estimations

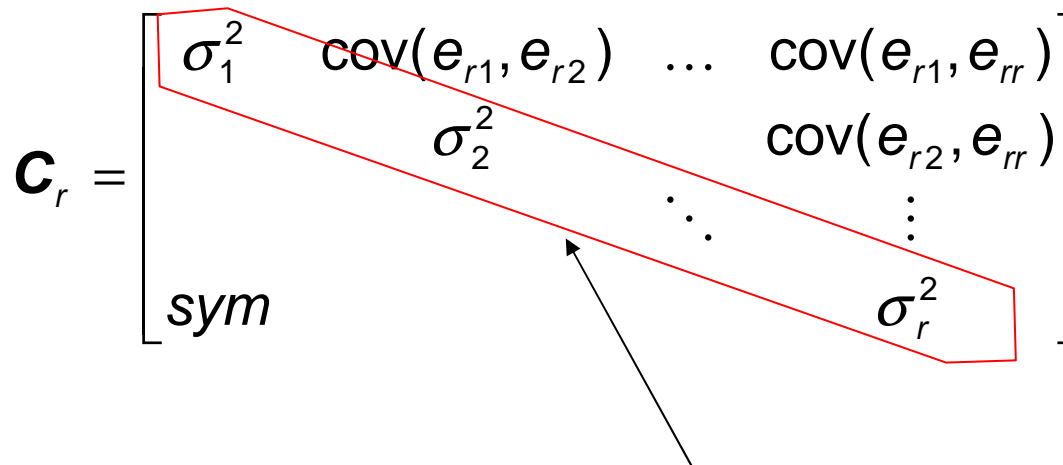
$$E[\mathbf{e}_{r2}] = -\mathbf{A}_r \mathbf{S}_c \mathbf{e}_c = [\mathbf{S}_r^t \mathbf{S}_r]^{-1} \mathbf{S}_r^t \mathbf{S}_c \mathbf{e}_c \neq 0$$

→ $[\mathbf{S}_r^t \mathbf{S}_r]^{-1} \mathbf{S}_r^t \mathbf{S}_c$ is a matrix ($r \times (n-r)$) that amplifies the bias on fixed parameters
(we have found another danger!)

For a fixed value of $\tilde{\mathbf{x}}_c$, the covariance matrix of estimations errors is

$$\mathbf{C}_r = \text{cov}(\mathbf{e}_r) = E[(\mathbf{e}_r - E[\mathbf{e}_r])(\mathbf{e}_r - E[\mathbf{e}_r])^t] = E[\mathbf{e}_{r1} \mathbf{e}_{r1}^t] = \text{cov}(\mathbf{e}_{r1}) = \mathbf{C}_1$$

The covariance matrix components are

$$\mathbf{C}_r = \begin{bmatrix} \sigma_1^2 & \text{cov}(e_{r1}, e_{r2}) & \dots & \text{cov}(e_{r1}, e_{rr}) \\ & \sigma_2^2 & & \text{cov}(e_{r2}, e_{rr}) \\ & & \ddots & \vdots \\ \text{sym} & & & \sigma_r^2 \end{bmatrix}$$


Individual variances on the r estimations are on the diagonal

$$\mathbf{c}_1 = [\mathbf{s}_r^t \mathbf{s}_r]^{-1} \sigma_\varepsilon^2$$

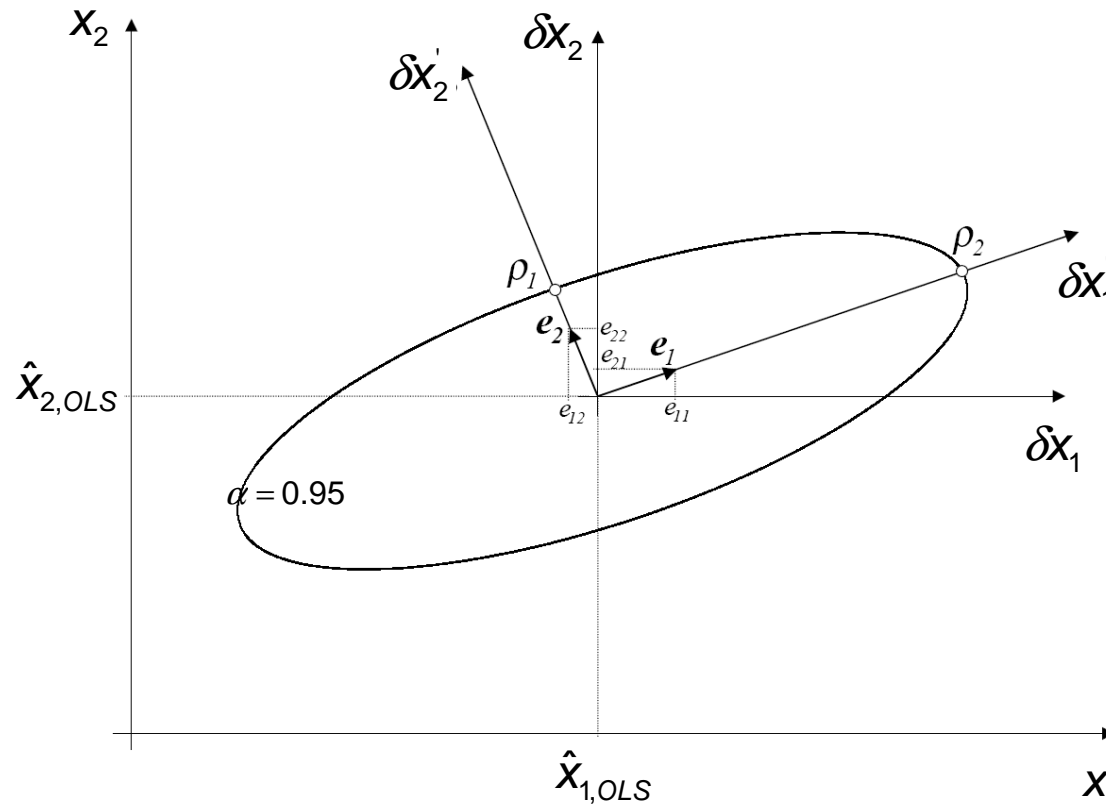
if σ_ε^2 is not measured before the experiment, an estimation of it may be obtained at the end of estimation thanks to the final value of the objective function :

$$J_{OLS}(\hat{\mathbf{x}}_{r,OLS}(\tilde{\mathbf{x}}_c)) = \sum_{i=1}^m r_i (\hat{\mathbf{x}}_{OLS}(\tilde{\mathbf{x}}_c))^2$$

a non biased estimation of σ_ε^2 for the estimation of r parameter from the use of m measurements is thus given by

$$\hat{\sigma}_\varepsilon^2 = \frac{J_{OLS}(\hat{\mathbf{x}}_{r,OLS}(\tilde{\mathbf{x}}_c))}{n-r}$$

Confidence ellipse at confidence level α



Equation in centered $(\delta x_1, \delta x_2)$ axes

$$\delta \mathbf{x}^t \cdot \mathbf{S}^t \mathbf{S} \cdot \delta \mathbf{x} = \Delta^2$$

$$\Delta^2 = \chi^2_{1-\alpha}(2) \sigma_\varepsilon^2$$

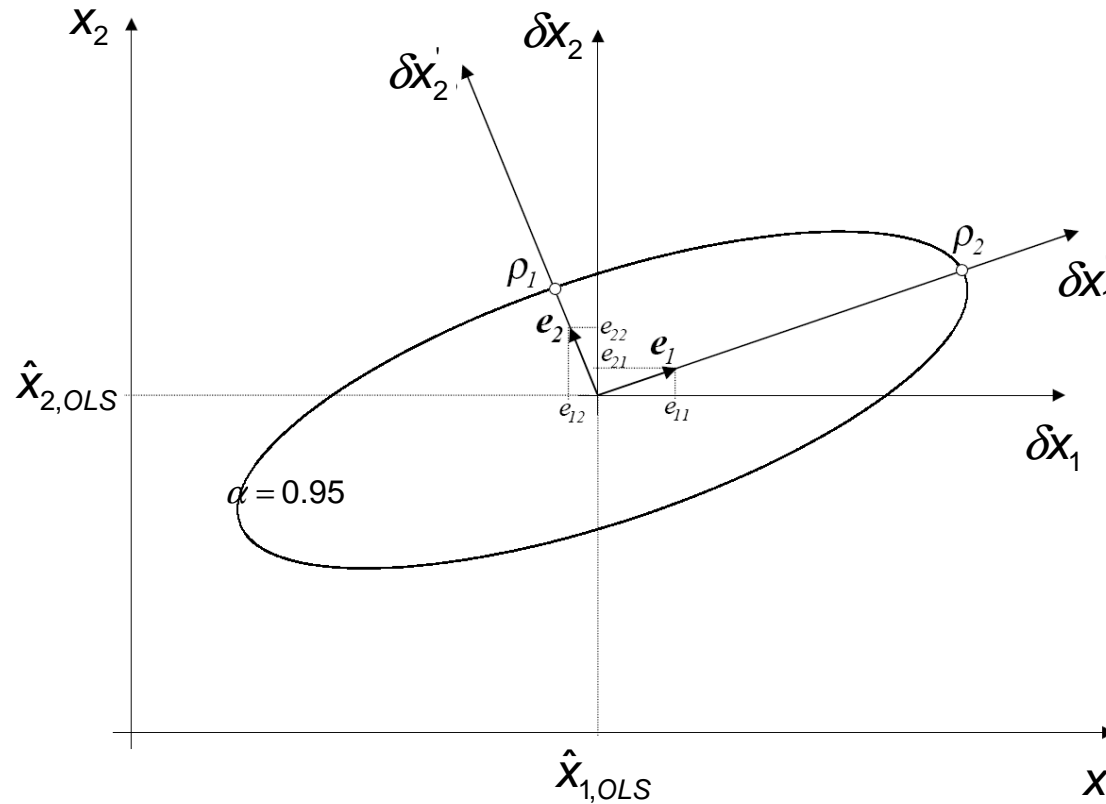
σ_ε^2 : variance of noise

$\chi^2_{1-\alpha}(2)$ is computed by `chi2inv(alpha,2)` in MATLAB[®] for a confidence region at a level 95% ($\alpha=0.95$)

Equation in principal axes $(\delta x'_1, \delta x'_2)$: $\delta \mathbf{x}'^t \cdot \mathbf{\Lambda} \cdot \delta \mathbf{x}' = \Delta^2$

Where $\mathbf{\Lambda} = \text{diag}(\lambda_1, \lambda_2)$ contains the eigenvalues of $\mathbf{S}^t \mathbf{S}$

Confidence ellipse at confidence level α



Length of the two half axis are 'long' if eigenvalues are 'small' :

$$\rho_1 = \Delta / \sqrt{\lambda_1}$$

$$\rho_2 = \Delta / \sqrt{\lambda_2}$$

Notice : determinant of $\mathbf{S}^t \mathbf{S}$
Is given by

$$\det(\mathbf{S}^t \mathbf{S}) = \lambda_1 \lambda_2$$

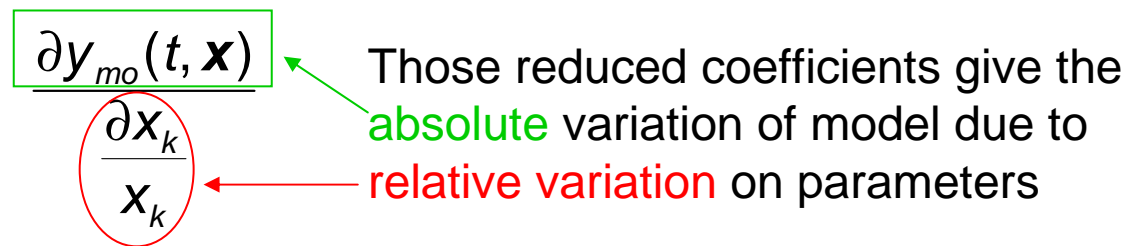
the area of the region inside the ellipse is given by

$$A = \pi \cdot \rho_1 \cdot \rho_2 = \frac{\pi \chi_{1-\alpha}^2 (2) \sigma_\varepsilon^2}{\sqrt{\det(\mathbf{S}^t \mathbf{S})}} = \frac{\pi \chi_{1-\alpha}^2 (2) \sigma_\varepsilon^2}{\sqrt{\lambda_1 \lambda_2}}$$

$\mathbf{C}_1 = [\mathbf{S}_r^t \mathbf{S}_r]^{-1} \sigma_\varepsilon^2$: 'absolute' covariance matrix of estimations

We can use $\mathbf{S}^* = \mathbf{S} \cdot \text{diag}(\mathbf{x})$ instead of \mathbf{S} , whose the columns contain the reduced sensitivity coefficients (of same unit than model y_{mo})

$$S_k^*(t, \mathbf{x}) = x_k S_k(t, \mathbf{x}) = x_k \left. \frac{\partial y_{mo}(t, \mathbf{x})}{\partial x_k} \right|_{t, x_j \text{ for } j \neq k} = \left. \frac{\partial y_{mo}(t, \mathbf{x})}{\frac{\partial x_k}{x_k}} \right|_{t, x_j \text{ for } j \neq k}$$



They can be compared between them and compared to the magnitude of noise

$$\mathbf{S}^* = \begin{bmatrix} S_1^*(t_1) & S_1^*(t_1) \\ \vdots & \vdots \\ S_i^*(t_i) & S_i^*(t_1) \\ \vdots & \vdots \\ S_m^*(t_m) & S_m^*(t_1) \end{bmatrix} = \begin{bmatrix} x_1 t_1 & x_2 \\ \vdots & \vdots \\ x_1 t_i & x_2 \\ \vdots & \vdots \\ x_1 t_m & x_2 \end{bmatrix}$$

With that reduced sensitivity matrix, we can build the **relative covariance matrix**

$$\mathbf{C}^* = \left[\mathbf{S}_r^{*t} \mathbf{S}_r^* \right]^{-1} \sigma_\varepsilon^2$$

$$\mathbf{C}^* = \begin{bmatrix} \left(\frac{\sigma_1}{\hat{x}_{1,OLS}} \right)^2 & \frac{\text{cov}(e_{r1}, e_{r2})}{\hat{x}_{1,OLS}^2} & \dots & \frac{\text{cov}(e_{r1}, e_{rr})}{\hat{x}_{1,OLS}^2} \\ & \left(\frac{\sigma_2}{\hat{x}_{2,OLS}} \right)^2 & & \frac{\text{cov}(e_{r2}, e_{rr})}{\hat{x}_{1,OLS}^2} \\ & & \ddots & \vdots \\ & & & \left(\frac{\sigma_r}{\hat{x}_{r,OLS}} \right)^2 \end{bmatrix}$$

sym

Relative standard deviation of each estimation!

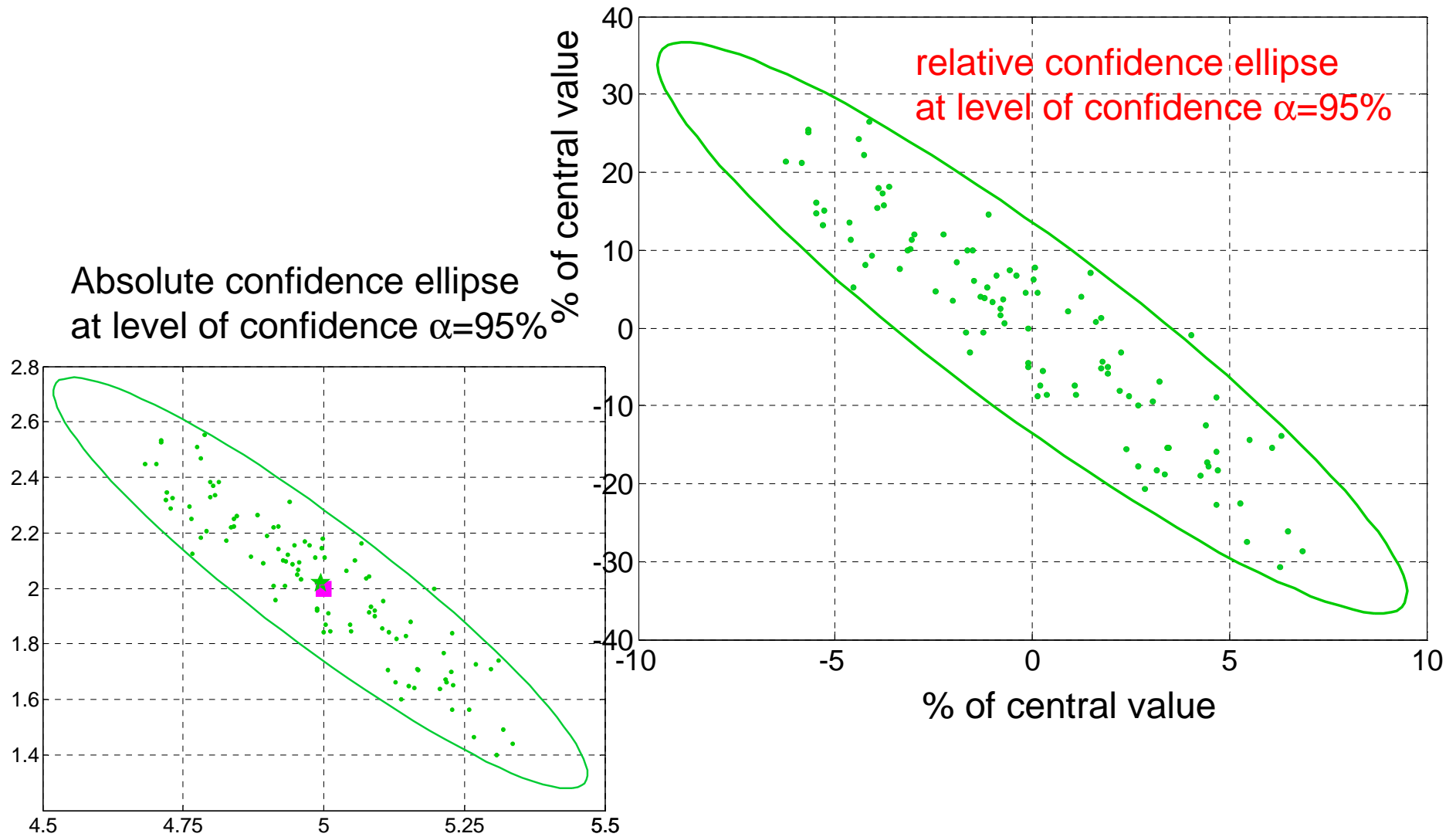
The same can be done with the ellipse equation

$$\delta \mathbf{x}^t \cdot \mathbf{S}^t \mathbf{S} \cdot \delta \mathbf{x} = \Delta^2$$

with $\mathbf{S}^* = \mathbf{S} \cdot \text{diag}(\mathbf{x}^{nom}) \rightarrow \mathbf{S} = \mathbf{S}^* \text{diag}(\mathbf{x}^{nom})^{-1}$

gives $\underbrace{\left(\text{diag}(\mathbf{x}^{nom})^{-1} \delta \mathbf{x} \right)^t}_{\frac{\delta \mathbf{x}}{\mathbf{x}^{nom}}} \cdot \mathbf{S}^t \mathbf{S} \cdot \text{diag}(\mathbf{x}^{nom})^{-1} \delta \mathbf{x} = \Delta^2$

$\frac{\delta \mathbf{x}}{\mathbf{x}^{nom}} \longrightarrow$ Relative confidence ellipse (in %)



Residuals analysis

Last, for qualifying the quality of estimation : the residuals analysis

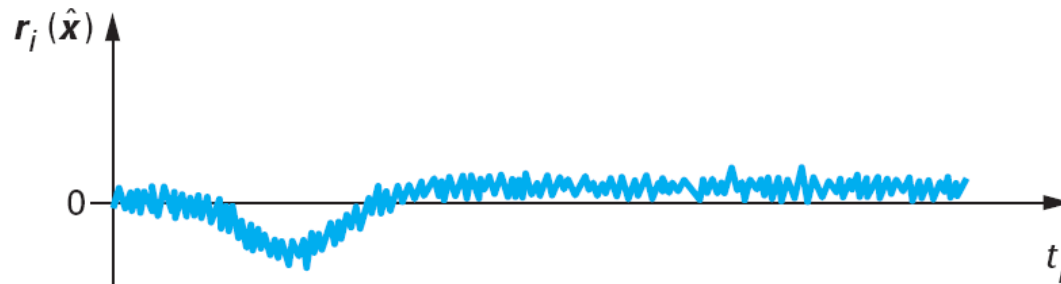
$$r(\hat{\mathbf{x}}) = \mathbf{y} - \mathbf{y}_{mo}(\hat{\mathbf{x}}) = [y_1 - y_{mo,1}(t_1, \hat{\mathbf{x}}) \quad \dots \quad y_i - y_{mo,i}(t_i, \hat{\mathbf{x}}) \quad \dots \quad y_m - y_{mo,m}(t_m, \hat{\mathbf{x}})]^t$$

Difference between measurements and model response with optimal parameters must 'look like' noise measurement : 'the right model with the right parameters must explain the measurements except its random part'



(a) Uncorrelated residuals

→ OK, see if the variances are not too large



(b) Signed residuals

→ Not OK : there may be a problem in the model or in the measurements

The danger has been identified : the inversion of $\mathbf{S}^t \mathbf{S}$ or $\mathbf{S}^{*t} \mathbf{S}^*$

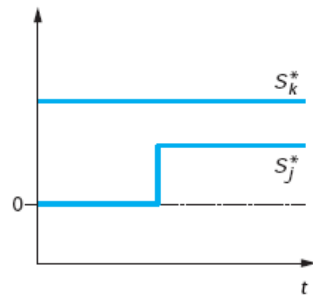
It has been shown that the matrix $\mathbf{S}^t \mathbf{S}$ is fundamental in the processus of parameter estimation :

- it has to be inverted to achieve the OLS estimation
- it also has to be inverted to compute the covariance matrix. The inverse of $\mathbf{S}^t \mathbf{S}$ respectively $\mathbf{S}^{*t} \mathbf{S}^*$ plays the role of "noise amplification", in absolute or, respectively, in relative values
- the eigenvalues of $\mathbf{S}^t \mathbf{S}$ enable the calculation of the lengths of the half principal axis of the elliptical confidence region
- the determinant of $\mathbf{S}^t \mathbf{S}$ enables the calculation of the area of the elliptical confidence region

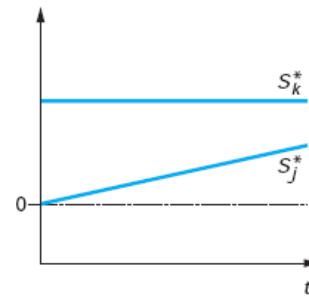
—————> Illustration in our examples, using too the conditioning number of $\mathbf{S}^t \mathbf{S}$

SENSITIVITY COEFFICIENTS composing \mathbf{S} MUST BE LINEARLY INDEPENDENT

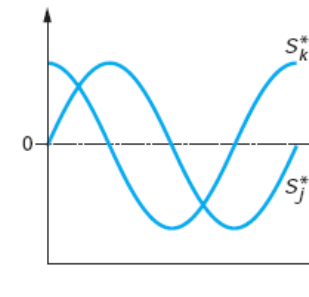
'Graphical' analysis of reduced sensitivity coefficients : independent case



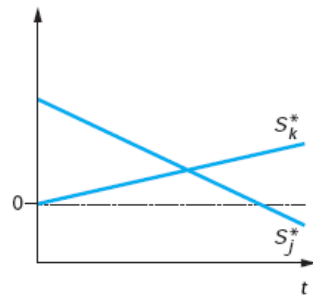
(a)



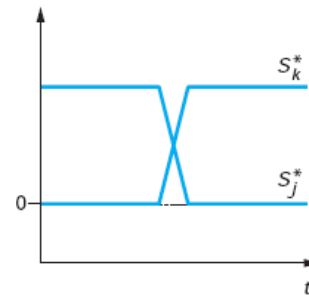
(b)



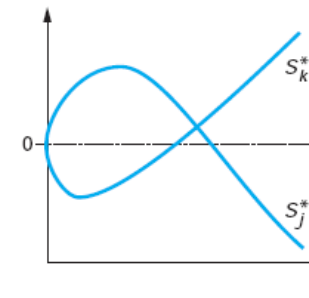
(c)



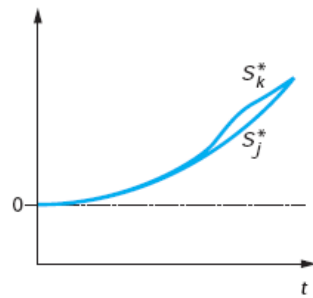
(d)



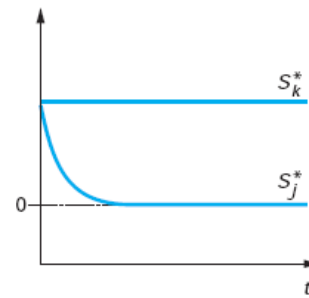
(e)



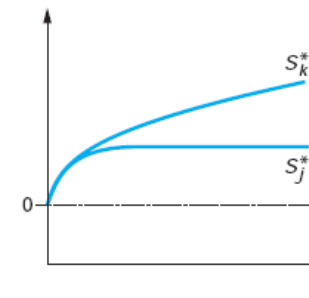
(f)



(g)

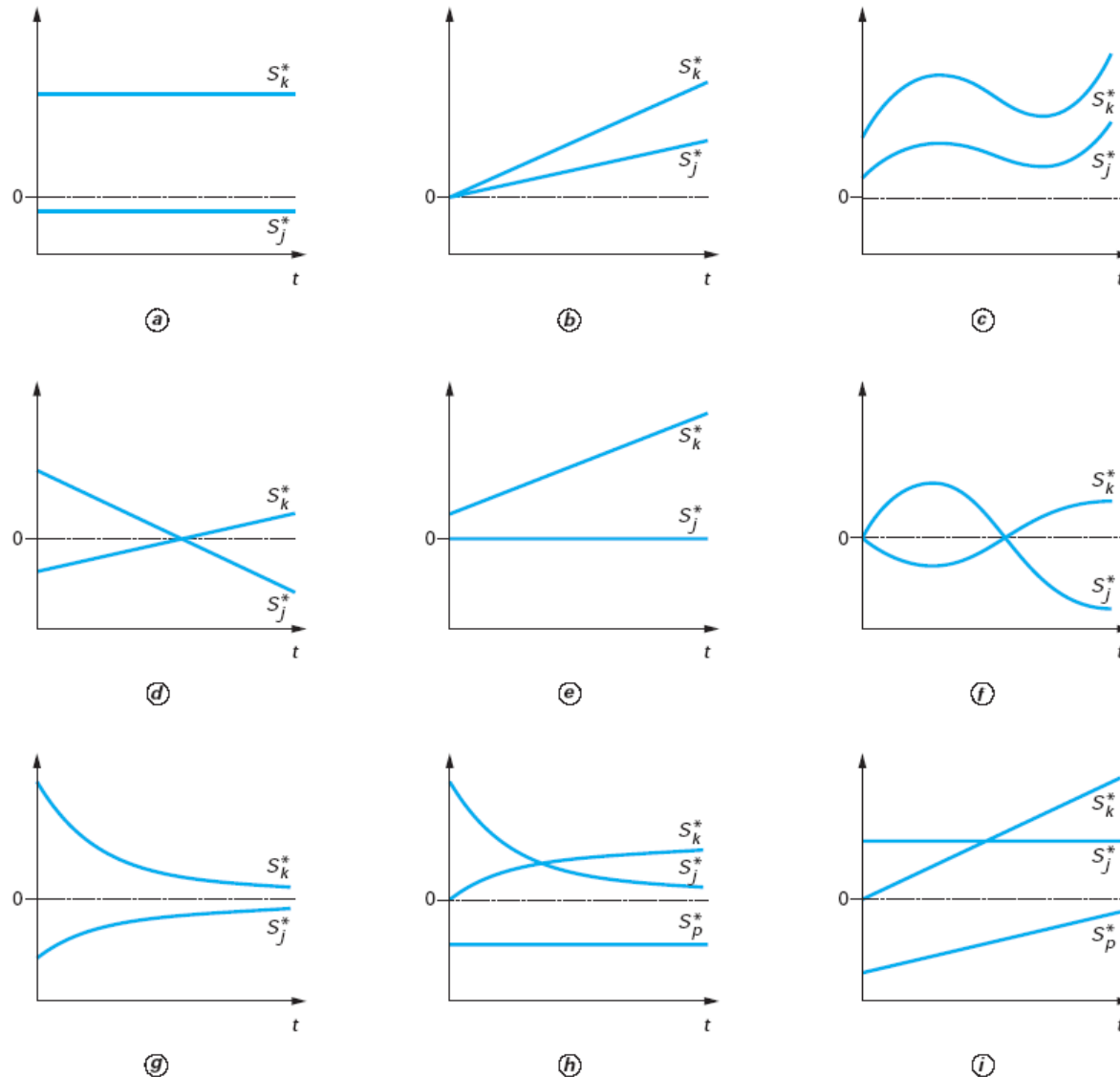


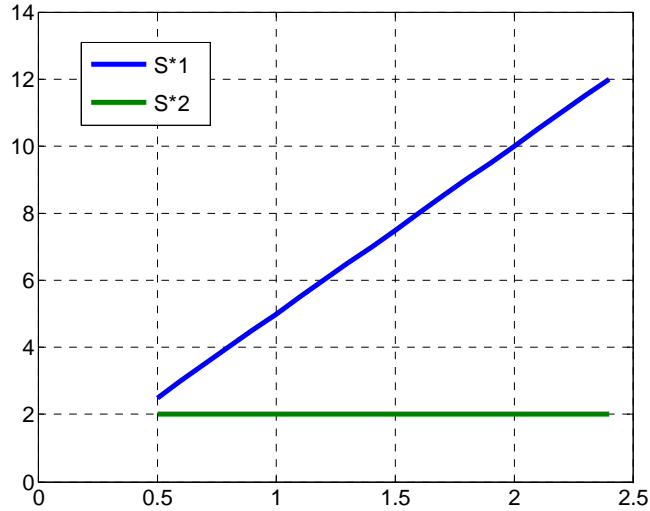
(h)



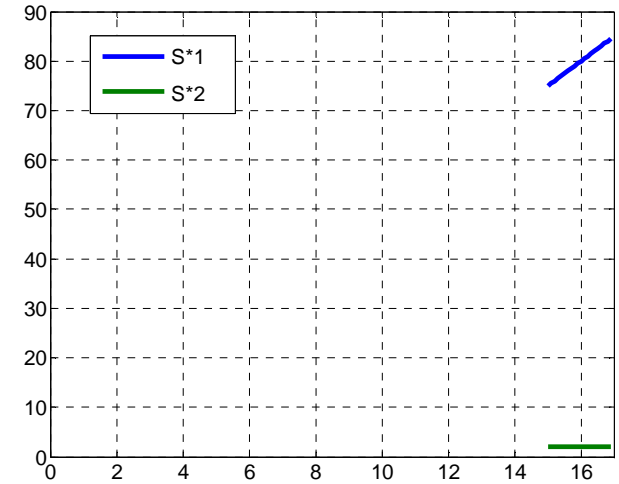
(i)

'Graphical' analysis of reduced sensitivity coefficients : dependent case

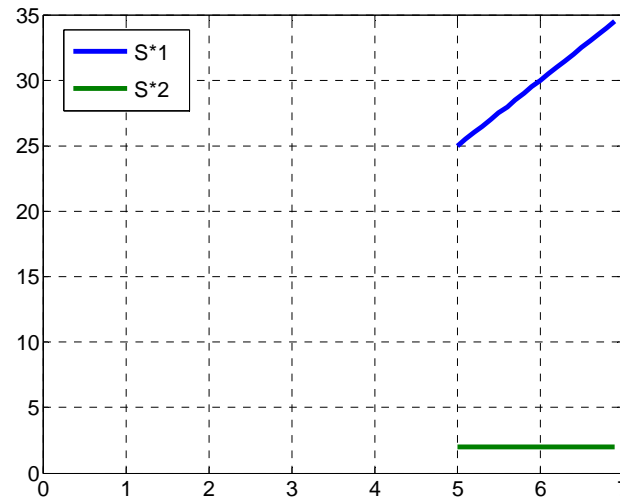




Student D.M.

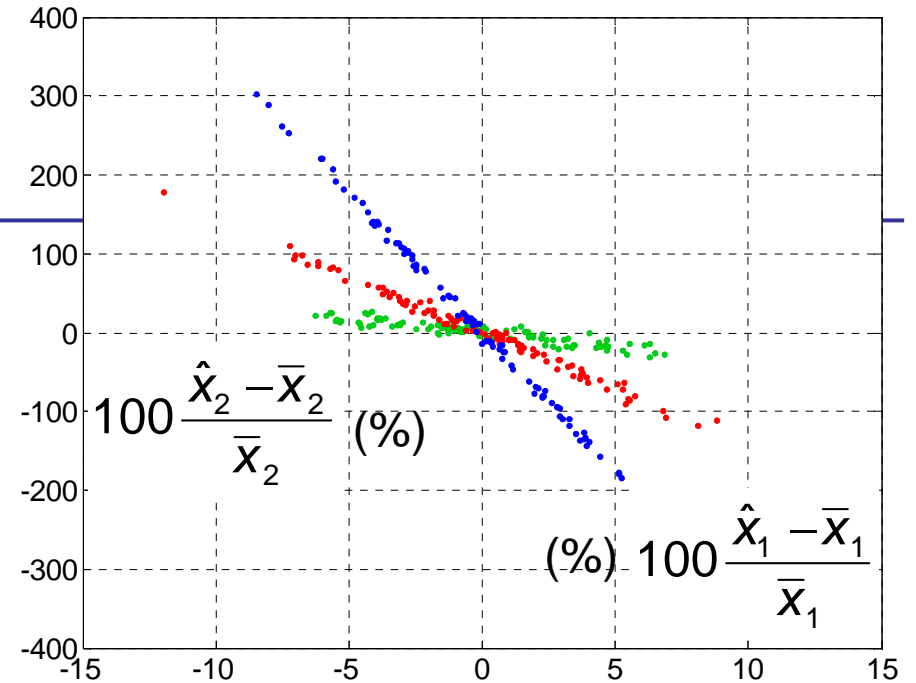
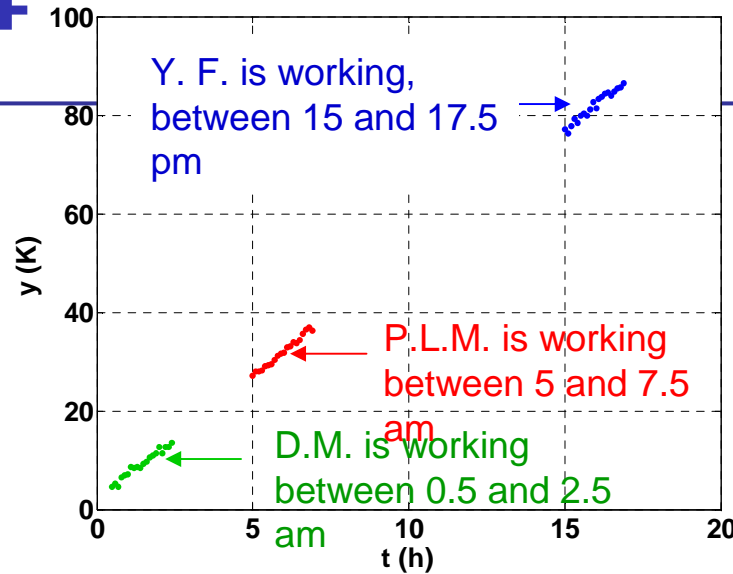


Student Y.F.



Student P.L.M.

Summary of Indicators



Student	D.M.	P.L.M.	Y.F.
Time range (h)	0.5 h -2.5 h	5 h -7.5 h	15 h -17.5 h
λ_{\min} of $\mathbf{S}^{*t} \mathbf{S}^*$ ↑	1.03e1	6.5e-1 ↓	6.2e-2 ↓
λ_{\max} of $\mathbf{S}^{*t} \mathbf{S}^*$ ↓	1.29e3	1.8e4 ↑	1.3e5 ↑
$\det(\mathbf{S}^{*t} \mathbf{S}^*)$ ↑	1.34e4	1.18e4 ↓	8.0e3 ↓
Ellipse area ↓	3.52e-4	3.99e-4 ↑	5.9e-4 ↑
$\text{cond}(\mathbf{S}^{*t} \mathbf{S}^*) = \lambda_{\max} / \lambda_{\min}$ ↓	1.24e2	2.78e4 ↑↑	2.1e6 ↑↑
ρ_{12} ↓	-0.93	-0.995 ↑	-0.993 ↔

All indicators are 'red' : it is not a good design to have large times for simultaneous estimation of x_1 and x_2