PEAS

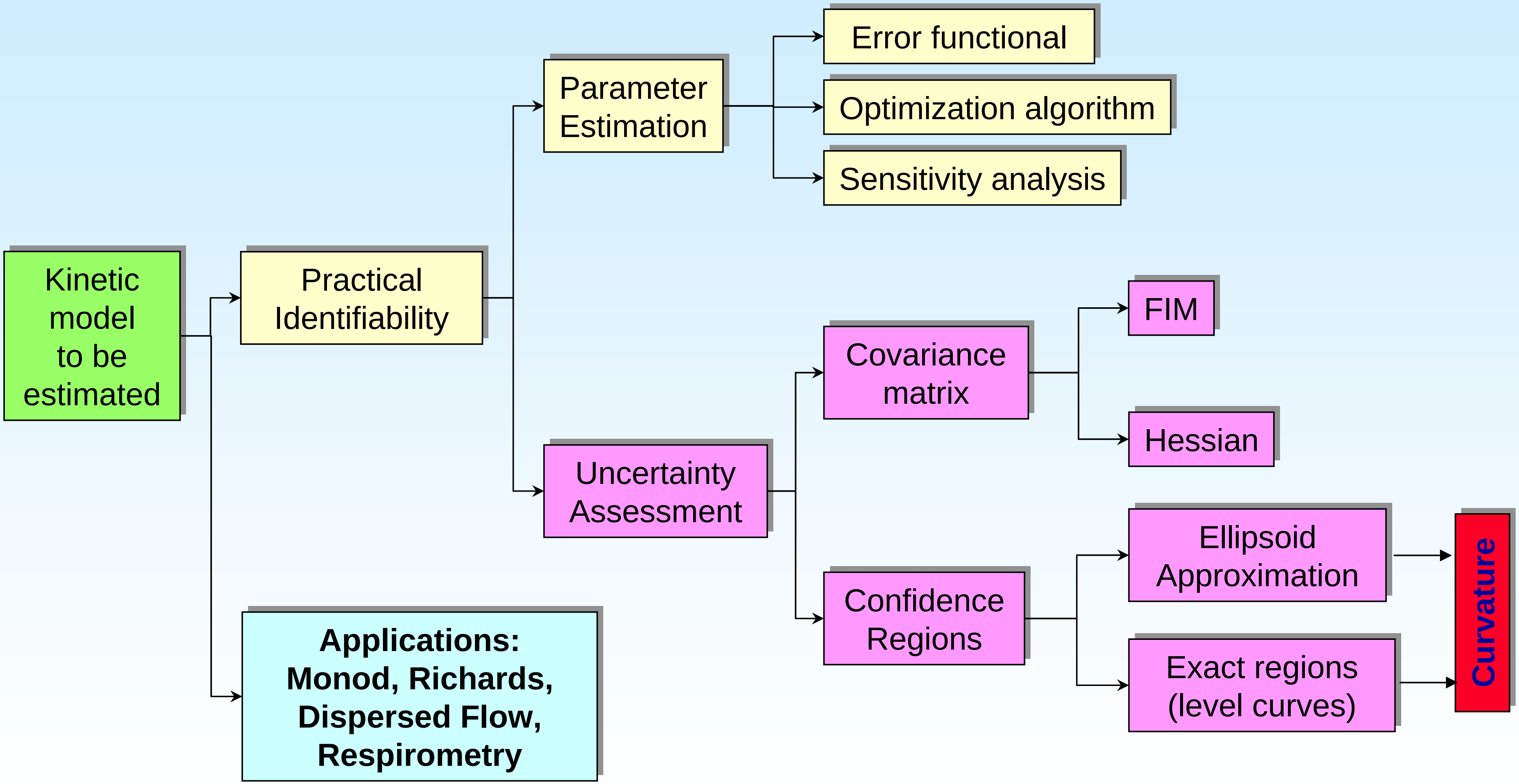
APPROXIMATE CONFIDENCE REGIONS IN THE ESTIMATION OF ECOLOGICAL MODELS PARAMETERS

Nicola Checchi, Elisabetta Giusti, and Stefano Marsili-Libelli
Department of Systems and Computers
University of Florence
ITALY

How it all started

- Our original goal was to associate ***confidence regions*** to estimated parameters
- We were looking for a numerical method to compute the ***approximate*** confidence regions
- Actually, we found ***two***….
  - Linear approximation based on sensitivity functions (FIM)
  - Second order approximation based on the Hessian matrix
- Plus…
  - A numerical method for computing the "exact" regions
- The different nature of the two approximation suggested an accuracy check
  - If the two regions coincide, the estimates can be considered ***accurate***
  - If they differ, the estimation should be considered ***critical***

Seminar material



Summary

- Confidence regions in a nutshell
  - Theory of confidence regions
  - A parameter estimation reliability test
- PEAS Implemented methods
  - Gridding
  - Trajectory sensitivity
  - Exact and approximate confidence regions
  - Radii criterion
  - Monte Carlo analysis
- PEAS software organization
  - Model implementation
- PEAS software demonstration
  - A dynamical simulation model
  - An algebraic model

Papers on parameters estimation

- The original paper on optimised simplex search for parameter estimation
  - Marsili-Libelli S. (1992). Parameter estimation of ecological models. ***Ecological Modelling*, 62**: 233-258.
- Confidence regions
  - Marsili-Libelli S., Guerrizio S., Checchi N. (2003). Confidence regions of estimated parameters for ecological systems. ***Ecological Modelling***, **165**: 127 - 146.
- Application to constructed wetland models
  - Marsili-Libelli, S. and Checchi, N., (2005). Identification of dynamic models for horizontal subsurface constructed wetlands. ***Ecological Modelling* 187**, 201 - 218.
- Application to respirometric models
  - Checchi, N, and Marsili-Libelli, S. (2005). Reliability of parameter estimation in respirometric models, ***Water Research* 39**, 3686 – 3696.
- This one
  - Checchi N., Giusti, E., Marsili-Libelli S. (2007). PEAS: a toolbox to assess the accuracy of estimated parameters in environmental models. ***Environmental Modelling & Software* 22,** *899 – 913.*
- Downloadable from: http://www.dsi.unifi.it/~marsili/recent.htm

Confidence regions

- Problem statement: find the minimum of the error functional

$$E(p) = \sum_{j=1}^{N} \left(y_j^{exp} - y_j(p)\right)^T V_j \left(y_j^{exp} - y_j(p)\right)$$

  - given the model

$$\begin{cases} \dfrac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p}) \\ \boldsymbol{y} = \boldsymbol{g}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p}) \end{cases}$$

- It is important to attach a ***measure of confidence*** to the estimates $\hat{\boldsymbol{p}}$
- For nonlinear in the parameters systems, only numerical methods are available

Confidence regions

- ☞ Determining the "best" parameter values is only a part of the estimation problem,
  - ✎ it is equally important to attach a ***measure of confidence*** to the estimates
- ☞ Most estimation techniques seek a ***valid*** set of parameters in terms of residuals, rather than a ***true*** model
- ☞ Many validation procedure involve model ***residuals*** and their ***correlation***
- ☞ For linear systems the exact confidence regions can be computed
- ☞ For nonlinear in the parameters systems, only numerical methods are available

Statement of the estimation problem

☞ Given a nonlinear system

$$\begin{cases} \dfrac{d\mathbf{x}}{dt} = \mathbf{h}(\mathbf{x},\mathbf{p},t) \\ \mathbf{y} = \mathbf{f}(\mathbf{x},\mathbf{p}) \end{cases} \qquad \begin{matrix} \mathbf{x} \in \Re^{n} \\ \mathbf{p} \in \Re^{n_p} \\ y \in \Re^{q} \end{matrix} \qquad \begin{matrix} \mathbf{h} : \Re^{n} \to \Re^{n} \\ \mathbf{f} : \Re^{n} \to \Re^{q} \end{matrix}$$

☞ and a quadratic error functional

$$E(\mathbf{p}) = \sum_{i=1}^{N} \left[\mathbf{y}_i^{s} - \mathbf{y}_i\right]^T \mathbf{V}_i^{-1} \left[\mathbf{y}_i^{s} - \mathbf{y}_i\right]$$

☞ Find the "best", in the LS sense, parameter vector $\hat{\mathbf{p}}$

$$\hat{\mathbf{p}} = \underset{\mathbf{p}}{arg\ min}\ E(\mathbf{p})$$

Estimation confidence regions

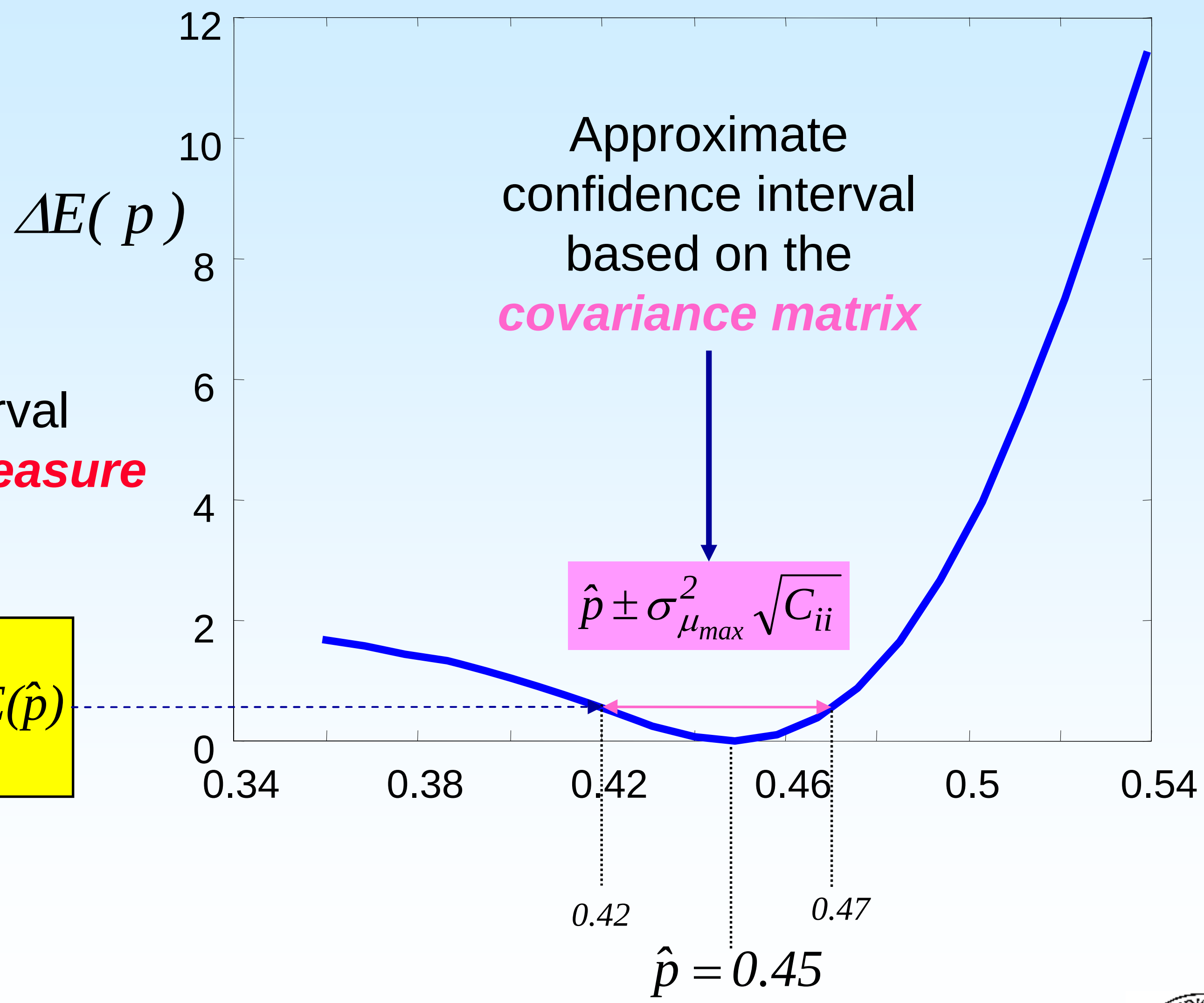
- ☞ Confidence regions provide a way to judge the accuracy of parameter estimates.
- ☞ Since the objective functional *E(**p**)* represents the "closeness" of the experimental data to the fitted model, it is justifiable to base the confidence region on its contours
- ☞ This is OK if you can find the ***contour level*** corresponding to a ***significant statistical level***

$$\left\{ \boldsymbol{p} : E(\boldsymbol{p}) \leq \left(1 + \frac{n_p}{N - n_p} F^{1-\alpha}_{n_p, N-n_p} \right) E(\hat{\mathbf{p}}) \right\}$$

Exact and approximate confidence intervals

Exact confidence interval
based on a ***statistical measure***

$$\left(1+\frac{n_p}{N-n_p}F^{1-0.95}_{n_p,N-n_p}\right)E(\hat{p})$$



Approximate confidence regions

☞ Confidence regions can be expressed as a function of the parameter covariance matrix $\boldsymbol{C}$

$$\left\{ \boldsymbol{p} : \left(\boldsymbol{p} - \hat{\mathbf{p}} \right)^T \boldsymbol{C}^{-1} \left(\boldsymbol{p} - \hat{\mathbf{p}} \right)^T \le n_p F_{n_p, N-n_p}^{1-\alpha} \right\}$$

☞ for a linear model $\boldsymbol{C}$ can be determined exactly

$$\boldsymbol{y} = \boldsymbol{p}\boldsymbol{x} + \boldsymbol{v} \quad \Rightarrow \quad \boldsymbol{C} = \sigma^2 \left(\boldsymbol{X}^T \boldsymbol{V}^{-1} \boldsymbol{X} \right)^{-1}$$

☞ For nonlinear models there is ***no exact way*** to obtain $\boldsymbol{C}$ and the linear approximation may yield a poor estimate of the real confidence region.

Approximations of covariance matrix

- ***Output linearisation (Jacobian)*** $C \rightarrow C_J$

$$C_J(\hat{\mathbf{p}}) = \frac{E(\hat{\mathbf{p}})}{N - n_p}\left(J^T V^{-1} J\right)^{-1} \quad J_{r,j}(\mathbf{p}) = \left.\frac{\partial f}{\partial p_j}\right|_{(x_r,\hat{\mathbf{p}})} = S_{p_j}^y$$

A link with sensitivity

- ***Fisher Information Matrix (FIM)***

$$FIM = \sum_{i=1}^{N}\left(\frac{\partial y_i}{\partial \mathbf{p}}\right)^T V_i^{-1}\left(\frac{\partial y_i}{\partial \mathbf{p}}\right)$$

If the residual distribution f is Gaussian and a LS estimator is used

$$C_J(\hat{\mathbf{p}}) = FIM^{-1}$$

The LS estimator yields a minimum variance result (Cramér-Rao lower limit).

- ***Error functional approximation (Hessian)*** $C \rightarrow C_H$

$$C_H(\hat{\mathbf{p}}) = \frac{2E(\hat{\mathbf{p}})}{N - n_p} H(\hat{\mathbf{p}})^{-1} \quad with \; H(\hat{\mathbf{p}}) = \left.\frac{\partial^2 E(\mathbf{p})}{\partial \mathbf{p} \partial \mathbf{p}^T}\right|_{\hat{\mathbf{p}}}$$

A link with the error functional shape

Hessian numerical approximation

Are C_J (FIM) and C_H the same thing?

NO, because

FIM

- Is based on a linear approximation
- Relies on sensitivity functions, hence is sensitive to the system output function
- Is dependent on output parametrisation

Hessian

- Is based on a second order approximation
- It depends on the error functional $E(\mathbf{p})$
- Is independent of output parametrisation

Component-wise….

$$\hat{\boldsymbol{H}}_{r,s} = 2\frac{N-n_p}{E(\hat{\mathbf{p}})}(\boldsymbol{FIM})_{r,s} - 2\sum_{i=1}^{N}\left[\left(\boldsymbol{y}_i^s - \boldsymbol{y}(\boldsymbol{x}_i,\hat{\mathbf{p}})\right)^T \boldsymbol{V}_i^{-1}\frac{d^2\boldsymbol{y}(\boldsymbol{x}_i,\hat{\mathbf{p}})}{dp_r dp_s}\right]$$

The ***curvature*** makes the difference

A digression on *curvature*

- Curvature is the distortion induced by parametric nonlinearities
- It can be defined as the second derivative of the surface generated by the output function

$$\Omega : \left\{ \boldsymbol{y}(t) = \varphi(\, \boldsymbol{x}, \boldsymbol{p}, t\,),\ \boldsymbol{p} \in \boldsymbol{P} \subset \Re^{n_p} \right\}$$

- $\boldsymbol{\Omega}$ is also called the *"expectation surface"* because it contains all the possible values of the output
- For a nonlinear system the shape of the surface $\boldsymbol{\Omega}$ may be heavily influenced by the curvature
- If the two representations do not agree, this means that the curvature term has significantly amplified the estimation error.

$$\left(\boldsymbol{y}_i^s - \boldsymbol{y}\left(\boldsymbol{x}_i, \hat{\boldsymbol{p}}\right)\right)^T \boldsymbol{V}_i^{-1} \frac{d^2 \boldsymbol{y}\left(\boldsymbol{x}_i, \hat{\boldsymbol{p}}\right)}{dp_r dp_s}$$

Estimation error → $\left(\boldsymbol{y}_i^s - \boldsymbol{y}\left(\boldsymbol{x}_i, \hat{\boldsymbol{p}}\right)\right)^T$

curvature → $\frac{d^2 \boldsymbol{y}\left(\boldsymbol{x}_i, \hat{\boldsymbol{p}}\right)}{dp_r dp_s}$

Components of curvature

- In the neighbourhood of $\hat{\boldsymbol{p}}$ curvature is composed of a ***tangent*** and a ***normal*** component with respect to the surface $\boldsymbol{\Omega}$
- The *tangent* component is the ***parameter curvature*** and represents the degree of curvature induced by the ***choice of parameters***
  - it can be reduced or eliminated by a proper re-parametrisation
- the *normal* component is the ***intrinsic curvature***: it measures the degree of distortion of the surface due to the ***nature of the output function in the solution space*** $y(t) = \varphi(\boldsymbol{x}, \boldsymbol{p}, t)$
  - it should become negligible around the minimum if the surface $\boldsymbol{\Omega}$ is well-behaved (i.e. almost flat) around $\hat{\boldsymbol{p}}$

Assessment of nonlinearity through curvature

- Through ***curvature*** the extent of model non-linearity can be assessed by comparing the maximum and minimum ***curvature radii***

$$r_{max} = (1 - \lambda_{max})^{-\frac{1}{2}} \quad r_{min} = (1 - \lambda_{min})^{-\frac{1}{2}}$$

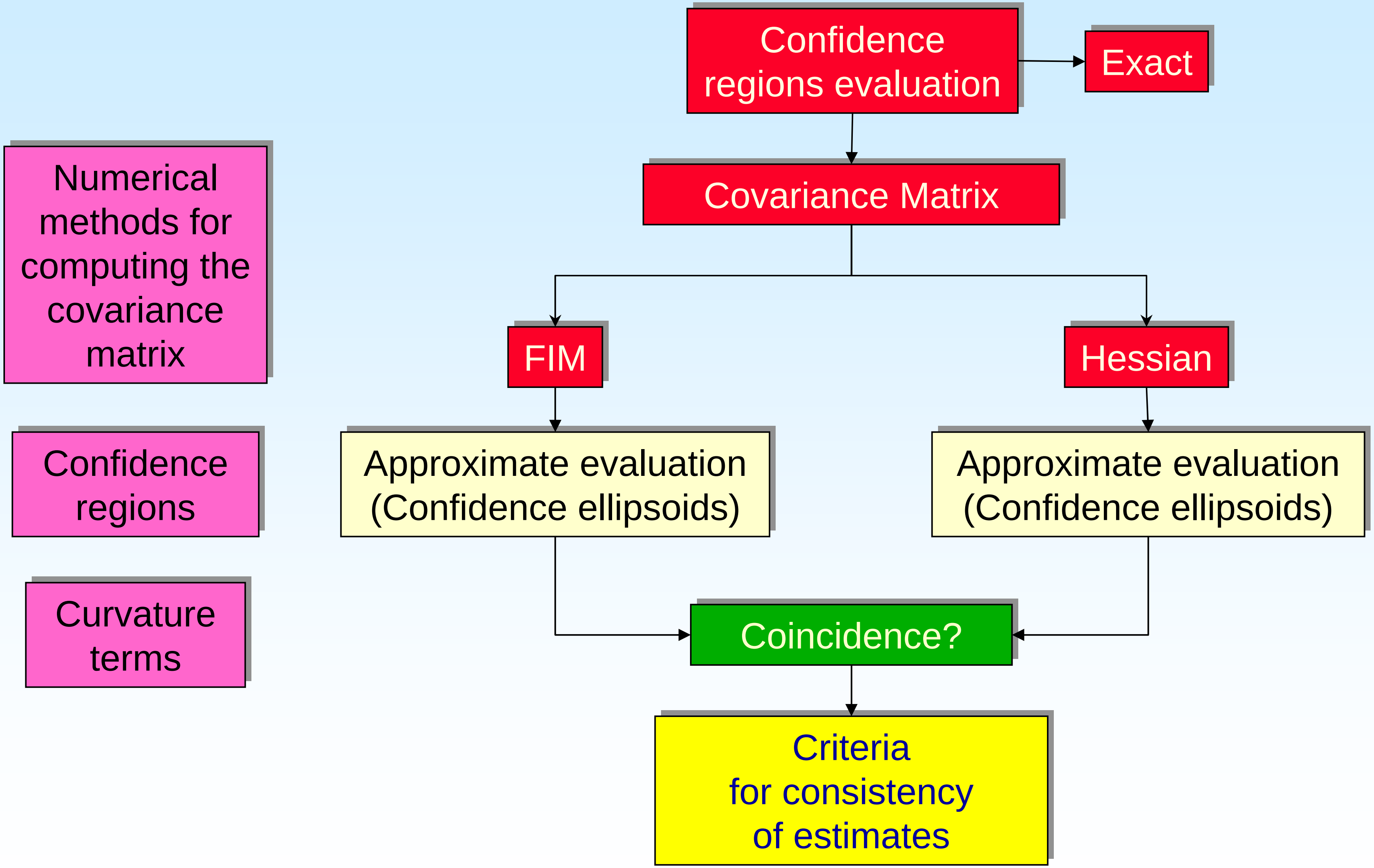
- where λ_{max} and λ_{min} are the extremal eigenvalues of the matrix ***B***, which relates the FIM and Hessian approximations

$$\boldsymbol{I}_{n_p} - \hat{\boldsymbol{B}} = \frac{1}{2} \hat{\boldsymbol{K}}^T \boldsymbol{H} \hat{\boldsymbol{K}}$$

- where ***H*** is the Hessian $\hat{\boldsymbol{K}} = \hat{\boldsymbol{R}}^{-1}$ and $\hat{\boldsymbol{R}}^T \hat{\boldsymbol{R}} \xrightarrow[Cholesky]{} \frac{\boldsymbol{FIM}}{s^2}$

- The closer r_{max} and r_{min} to 1, the smaller is the curvature

Method summary



Approximate confidence regions as discriminators

FIM approximation

$$\left\{ \mathbf{p} : (\mathbf{p}-\hat{\mathbf{p}})^T \hat{\mathbf{J}}_n^{\,T} \mathbf{V}^{-1} \hat{\mathbf{J}}_n (\mathbf{p}-\hat{\mathbf{p}}) \le s^2 n_p F^{1-\alpha}_{n_p, N-n_p} \right\}$$

YES

Reliable estimates

Exact confidence regions

$$\left\{ \mathbf{p} : E(\mathbf{p}) \le cE(\hat{\mathbf{p}}) \right\} \qquad c > 1$$

Coincident regions?

NO

Doubtful estimates

Hessian approximation

$$\left\{ \mathbf{p} : (\mathbf{p}-\hat{\mathbf{p}})^T \mathbf{H}_n (\mathbf{p}-\hat{\mathbf{p}}) \le s^2 n_p F^{1-\alpha}_{n_p, N-n_p} \right\}$$

Curvature effect

$$\left[\left(\frac{\partial^2 \boldsymbol{f}(\boldsymbol{p})}{\partial p_r \partial p_s}\right)\right]_{\hat{\mathbf{p}}} = \left[\left(\hat{\boldsymbol{f}}_{rs}\right)\right] \in \Re^{N\times n_p \times n_p}$$

Accounts for the quadratic terms neglected in the output function linearisation

Parametric
$\boldsymbol{f}$ tangent component @ $\hat{\boldsymbol{p}}$

Can be reduced through adequate re-parametrisation

Intrinsic
$\boldsymbol{f}$ normal component @ $\hat{\boldsymbol{p}}$

Independent from parameter choice

Evaluate *max* and *min* curvature radii

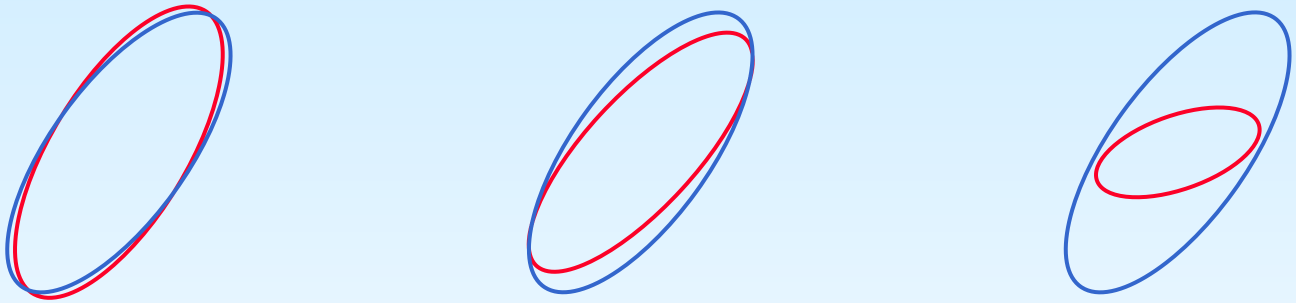
Radii close to unity indicate reliable linearisation

Distortion effect of the output solution space

$$\boldsymbol{y}(t) = \varphi(\boldsymbol{x}, \boldsymbol{p}, t)$$

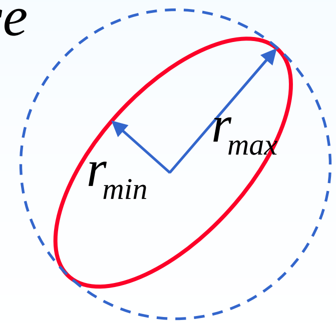
A less subjective test

- Judging ellipses misalignment involves a good deal of subjectivity



good agreement suspect agreement poor agreement

- The new test is based on the distortion induced by the curvature, i.e. how much the ellipse differs from a sphere
  - The curvature is responsible for the distortion *in the transformed space*



$$\rho = \frac{r_{max}}{r_{min}} \rightarrow 1$$ in the perfect case

Assessment of nonlinearity through curvature

- Through ***curvature*** the extent of model non-linearity can be assessed by comparing the maximum and minimum ***curvature radii***

$$r_{max} = (1 - \lambda_{max})^{-\frac{1}{2}} \quad r_{min} = (1 - \lambda_{min})^{-\frac{1}{2}}$$

- where λ_{max} and λ_{min} are the extremal eigenvalues of the matrix ***B***, which relates the FIM and Hessian approximations

$$\boldsymbol{I}_{n_p} - \hat{\boldsymbol{B}} = \frac{1}{2} \hat{\boldsymbol{K}}^T \boldsymbol{H} \hat{\boldsymbol{K}}$$

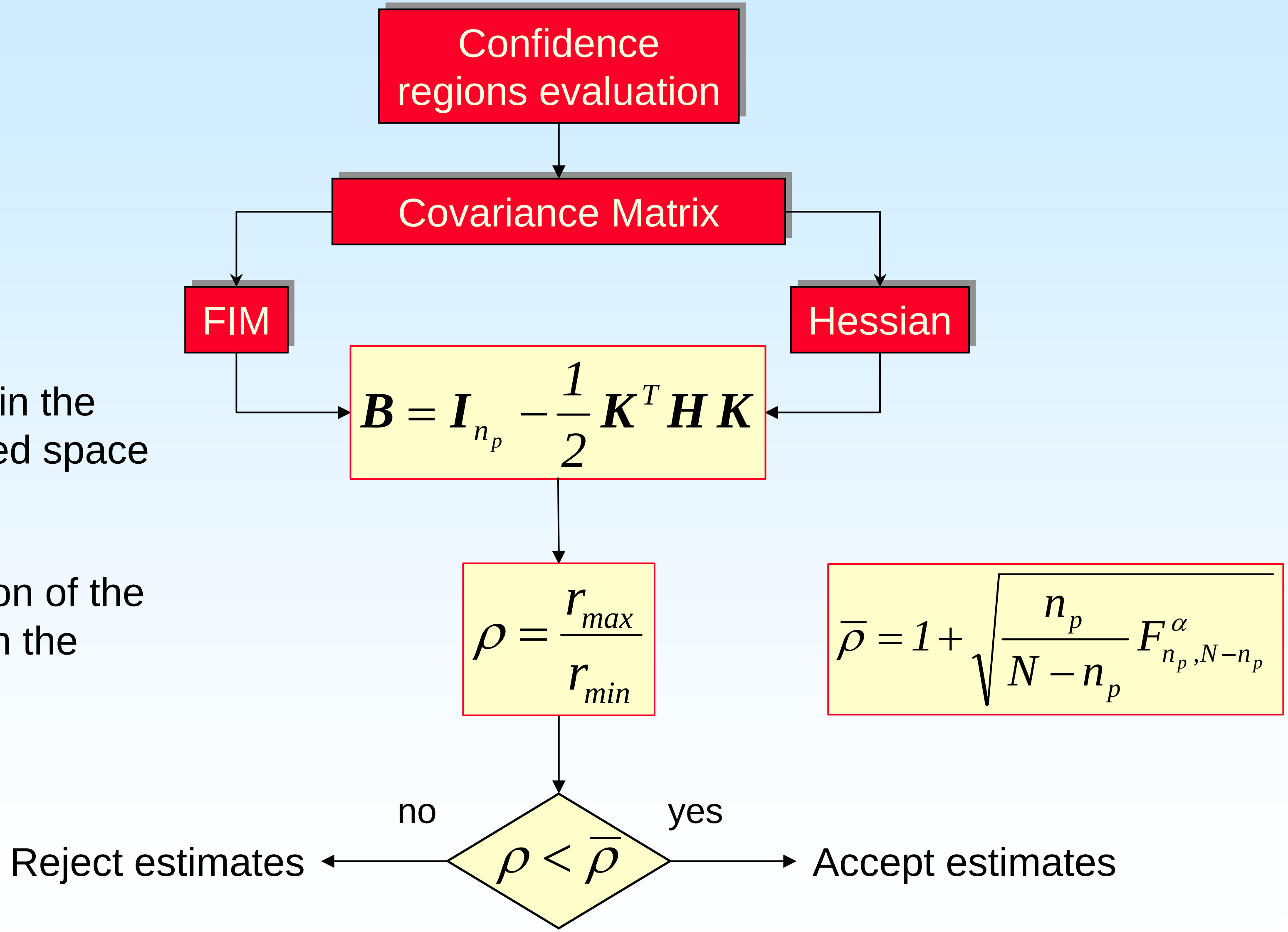
- where ***H*** is the Hessian $\hat{\boldsymbol{K}} = \hat{\boldsymbol{R}}^{-1}$ and $\hat{\boldsymbol{R}}^T \hat{\boldsymbol{R}} \xrightarrow[Cholesky]{} \frac{\boldsymbol{FIM}}{s^2}$

- The radii criterion is obtained $\overline{\rho} = 1 + \sqrt{\frac{n_p}{N - n_p} F^{\alpha}_{n_p, N-n_p}}$

Method summary

Distortion in the transformed space

Comparison of the ratio ρ with the threshold

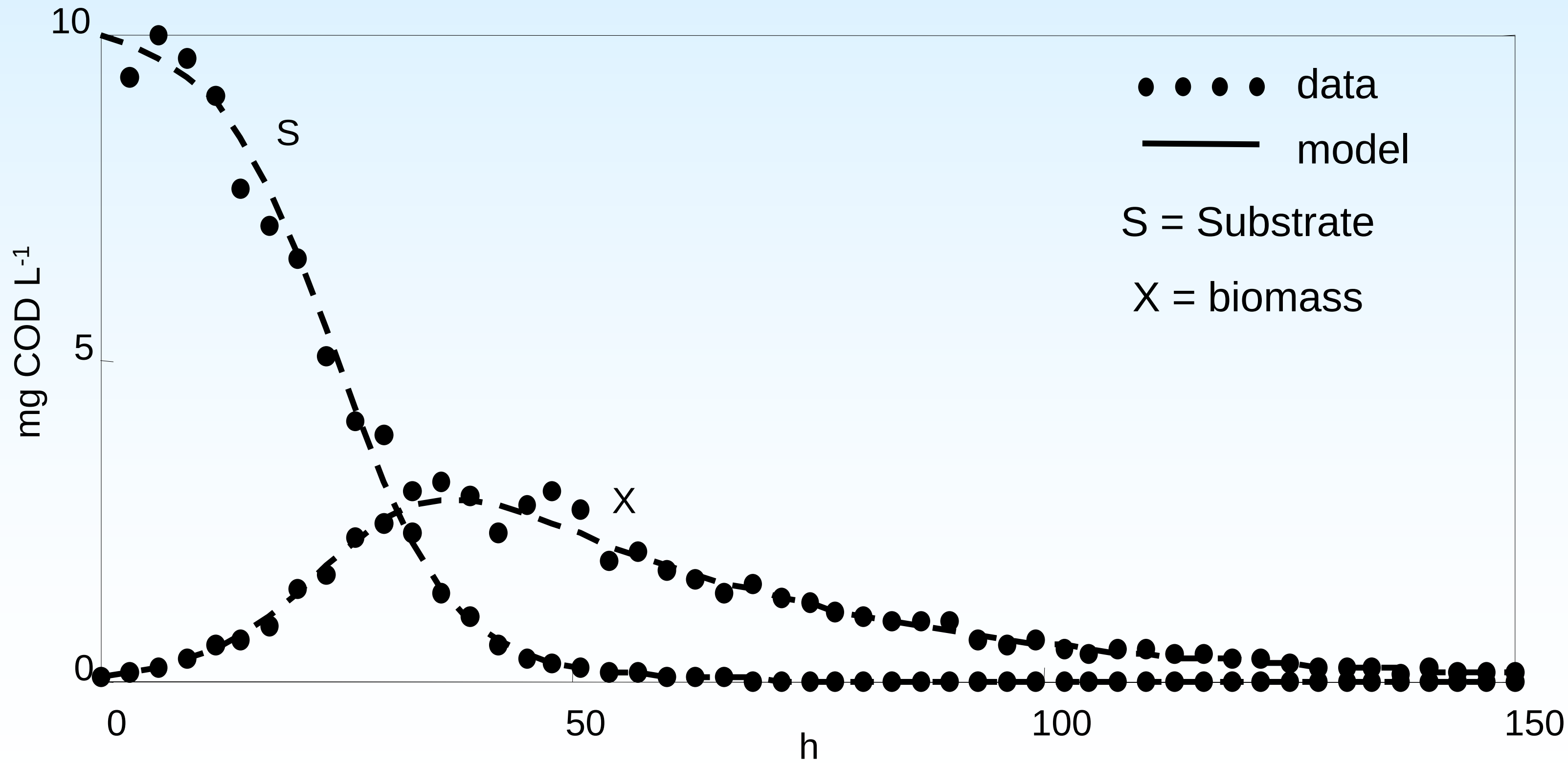


Applications

- **Ecological Kinetics**
  - Monod
  - Richards
    - ***Identification difficulty induced by the shape of the error functional***
    - ***Importance of proper initialisation***
- **Dispersed flow modelling**
  - Horizontal subsurface constructed wetlands (HSCW)
    - ***Model selection assessment***
- **Respirometry**
  - Reliability of estimation of a two-step nitrification model
  - Influence of the initial Ammonium-N injection on identifiability
    - ***Selection of critical parameters (second step)***

Monod kinetics

- Well known estimation difficulties
  - Strong parameters correlation
- Test with synthetic noisy data
- Both substrate and biomass observed



Estimation results for the Monod kinetics

Model

$$\begin{cases} \dfrac{dS}{dt} = -\dfrac{1}{Y}\dfrac{\mu_{max} S}{K_s + S} X \\ \dfrac{dX}{dt} = \dfrac{\mu_{max} S}{K_s + S} X - K_d X \\ \mathbf{x} = [S \ X]^T \quad \mathbf{y} = \mathbf{x} \end{cases}$$

$S(0) = 10 \ mg/L \qquad X(0) = 0.1 \ mg/L$

$\bar{\mathbf{p}} : \mu_{max} = 0.5 \ (h^{-1}); \ K_s = 20 \ (mg \ COD.L^{-1}); \ Y = 0.5; \ K_d = 0.03 \ (h^{-1})$

Estimation from noisy data (σ = 0.05)

	$K_s \left(mg\,COD\,L^{-1}\right)$	$\mu_{max}\left(h^{-1}\right)$	Y	$K_d\left(h^{-1}\right)$	**Starting point**	$E(\hat{\mathbf{p}})$
True values	20.000	0.500	0.500	0.0030		
Case 1	19.0997	0.483	0.525	0.0303	$[22.0 \ 0.5 \ 0.37 \ 0.04]^T$	0.265
Case 2	31.605	0.711	0.485	0.0289	$[33.3 \ 0.8 \ 0.57 \ 0.08]^T$	0.548

Case 1: Search successfully terminates at the minimum

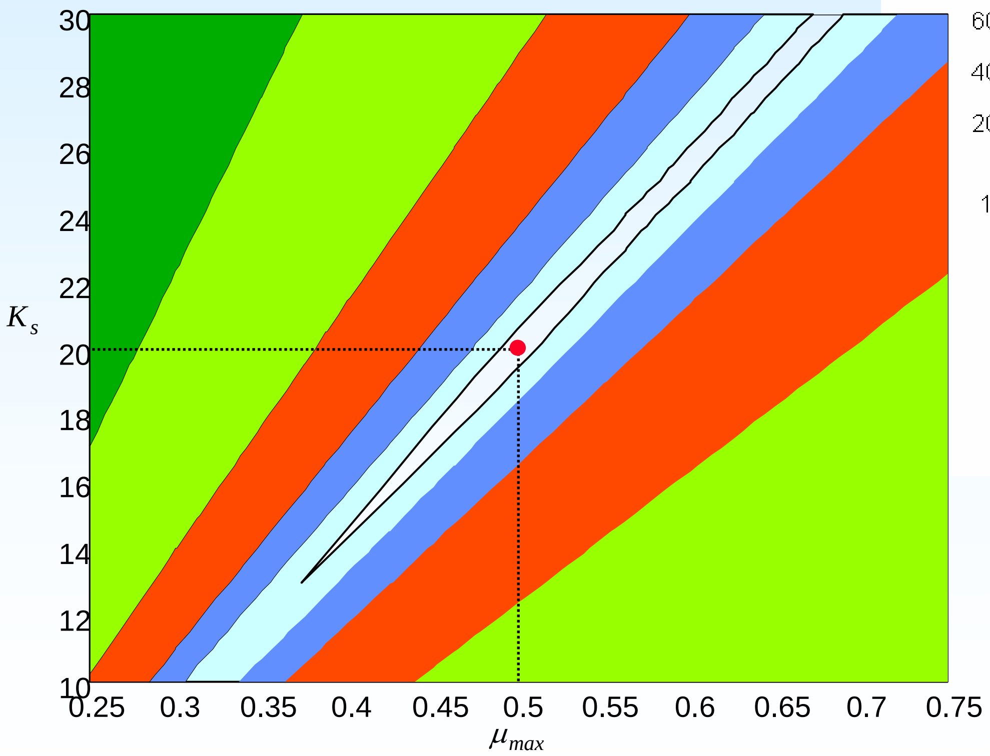
Case 2: Search terminates at a wrong point, because of unsuitable initialisation

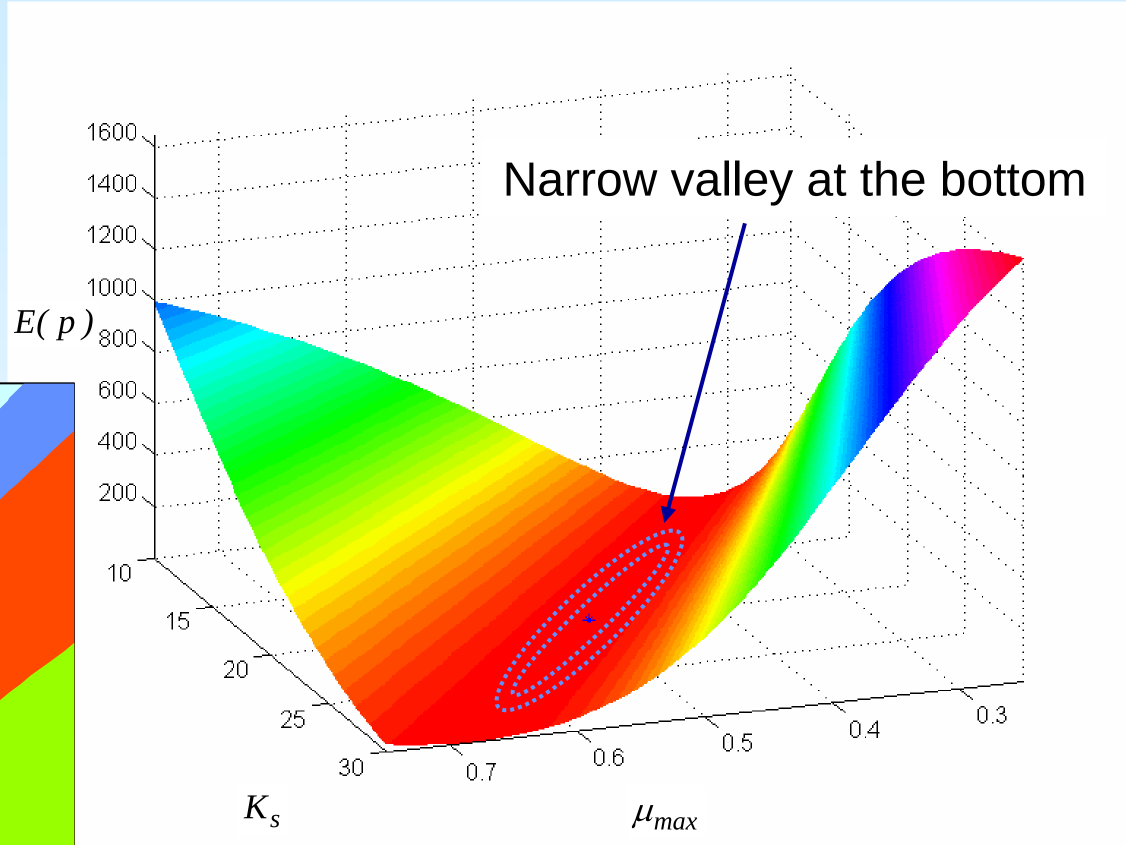
Confidence intervals

	$K_s\left(mg\,COD\,L^{-1}\right)$	$\mu_{max}\left(h^{-1}\right)$	Y	$K_d\left(h^{-1}\right)$
Case 1	19.09968 ± 1.72181	0.48298 ± 0.03212	0.50524 ± 0.01139	0.03025 ± 0.00057
True values	20.000	0.5000	0.5000	0.0030

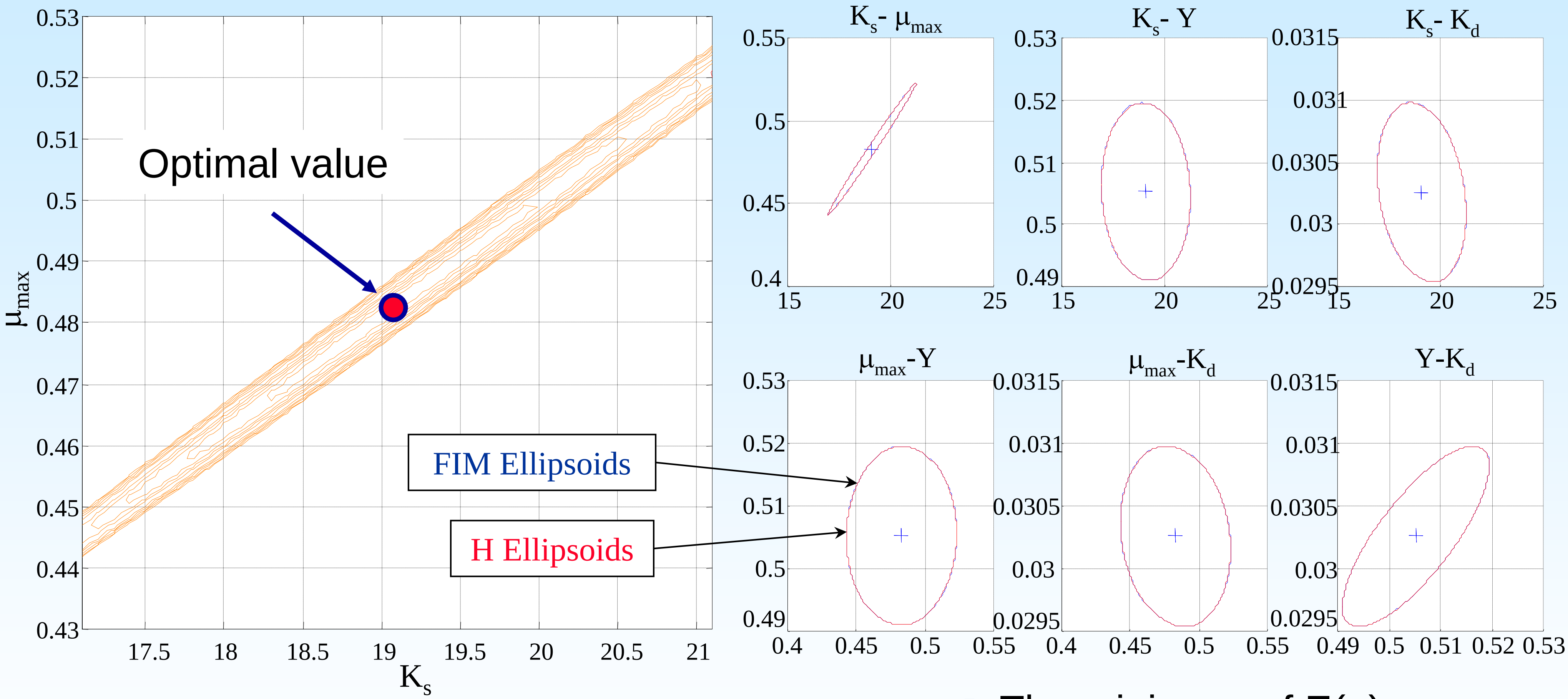
- ☞ K_s, with a 95% confidence interval of over **18 %** of the estimated value, has the largest uncertainty, though much less than that found by Holmberg (1982)
- ☞ μ_{max} has a 13 % uncertainty
- ☞ Y has a 4.4 % uncertainty
- ☞ K_d only 3.8 %.

Shape of E(p) for the Monod kinetics





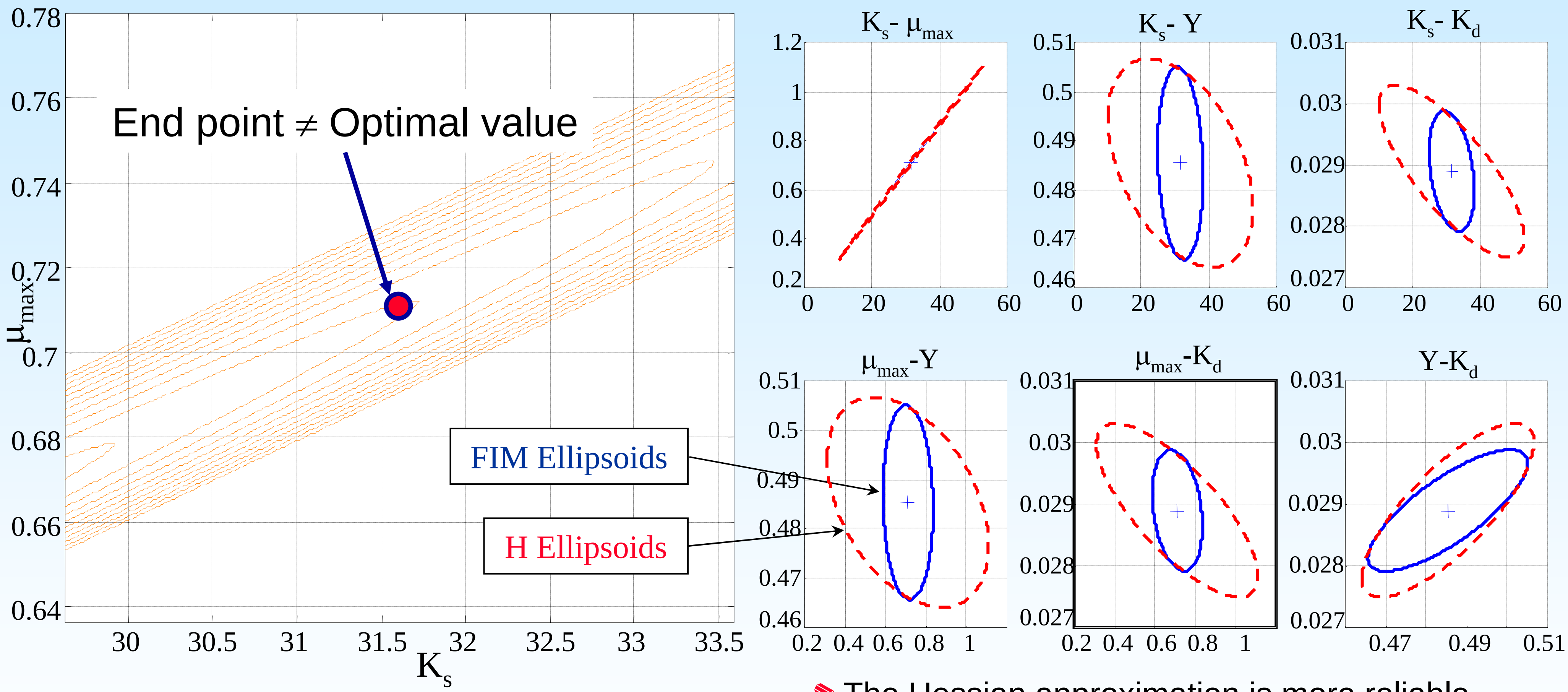
Case (1): E(p) minimum reached



The two ellipsoids coincide and include the exact parameters

- ➔ The minimum of E(p) was reached
- ➔ Reliability of linearisation
- ➔ No curvature effects

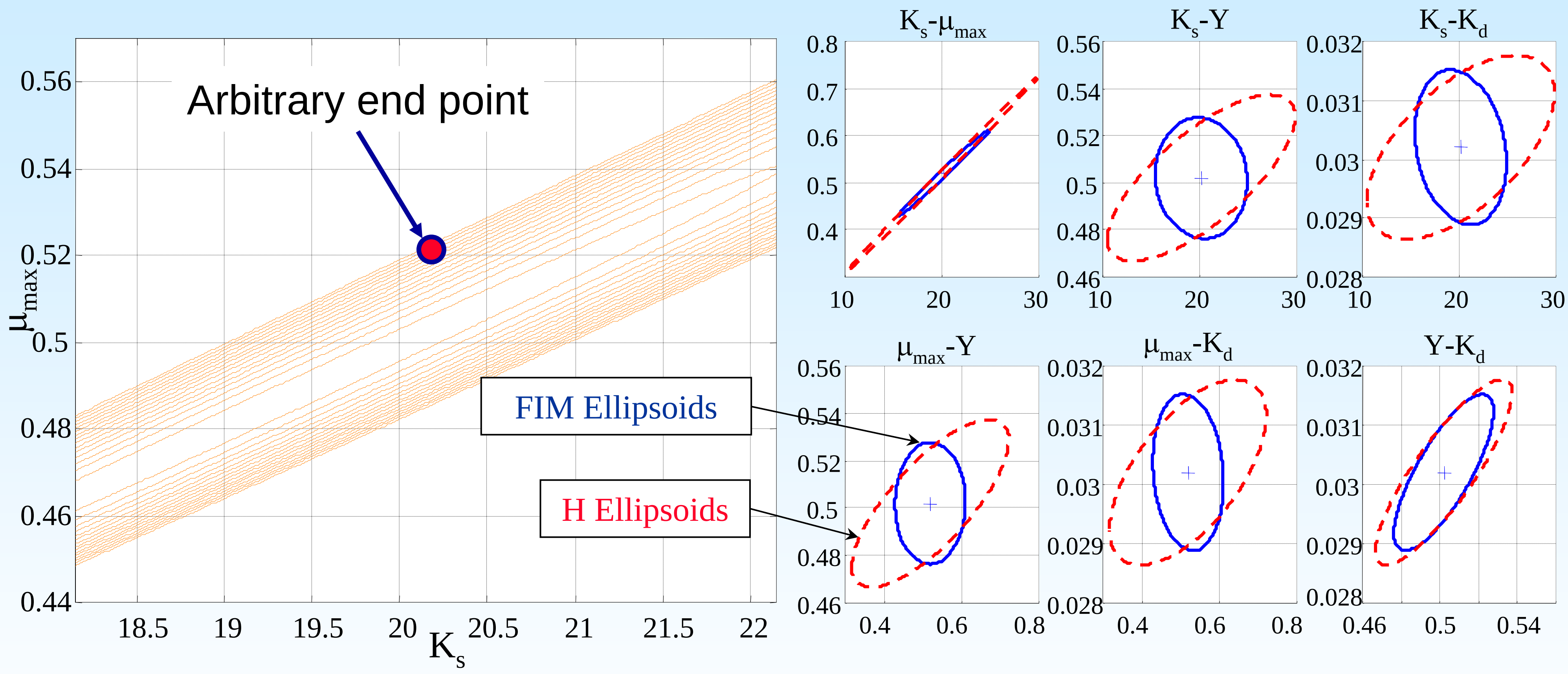
Case (2): E(p) minimum not reached but still in the valley



Only the Hessian approximation includes the exact values, because it conforms to the shape of E(p)

- The Hessian approximation is more reliable
- The H and J ellipses have axes with differing slopes, hence indicate differing parameter correlations

Case (3): the end point is not in the valley



Both approximations are unreliable

➔E(p) gradient not negligible

➔Curvature effect is relevant

Curvature radii

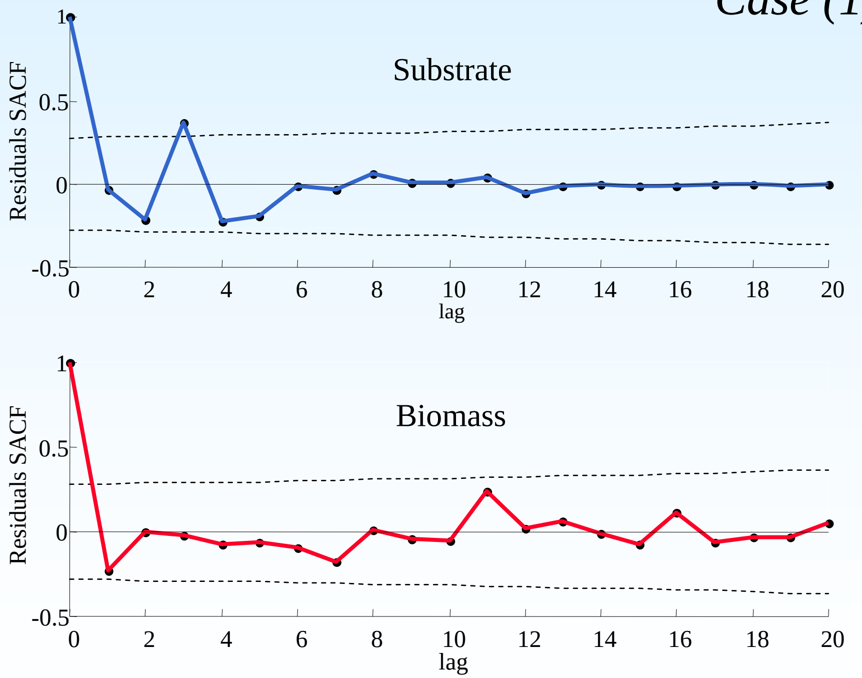
Minimum and maximum curvature radius
for the two Monod calibration cases

	r_{min} - r_{max}		
	μ_{max}	Y	K_d
K_s	Case 1: 0.9961 - 1.0009 Case 2: 0.9668 – 2.9963	Case 1: 0.9996 - 1.0004 Case 2: 0.9723- 1.1780	Case 1: 0.9988 - 1.0004 Case 2: 0.9698- 1.4414
μ_{max}	---	Case 1: 0.9966 - 0.9998 Case 2: 0.9925 – 3.0541	Case 1: 0.9964 - 0.9991 Case 2: 0.9578 – 3.1749
Y	---	---	Case 1: 0.9988 - 0.9998 Case 2: 0.9908 – 1.5607

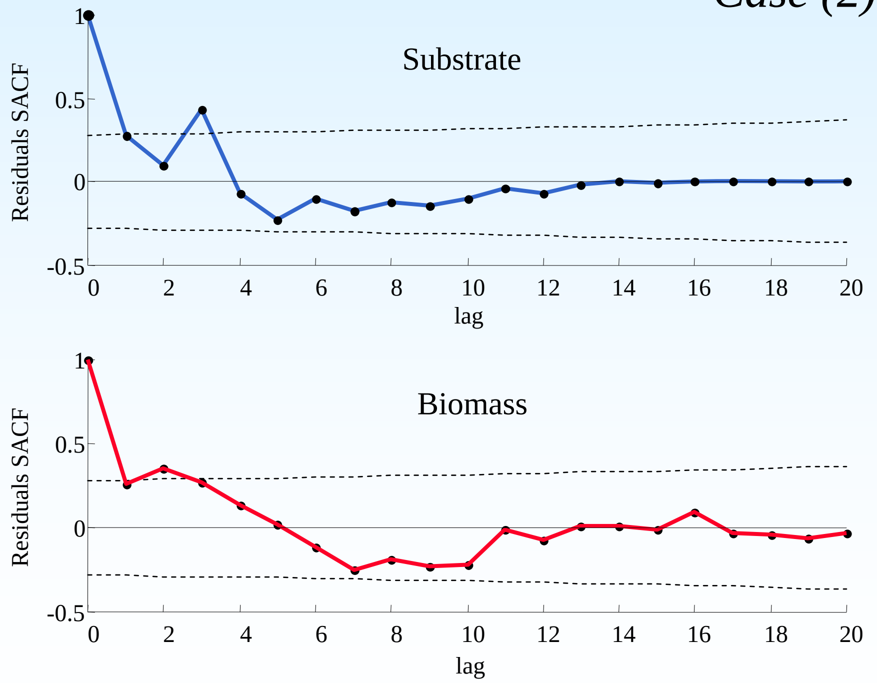
Residual autocorrelation (RAC)

- ✓ Even Case 1 yields partially correlated residuals
- ✓ Though Case 2 performs slightly worse, it is hard to discriminate
- ✓ In both cases, some samples fall outside the zero-confidence limit
- ✓ The discriminatory power of RAC is much less than confidence ellipsoids.

Case (1)

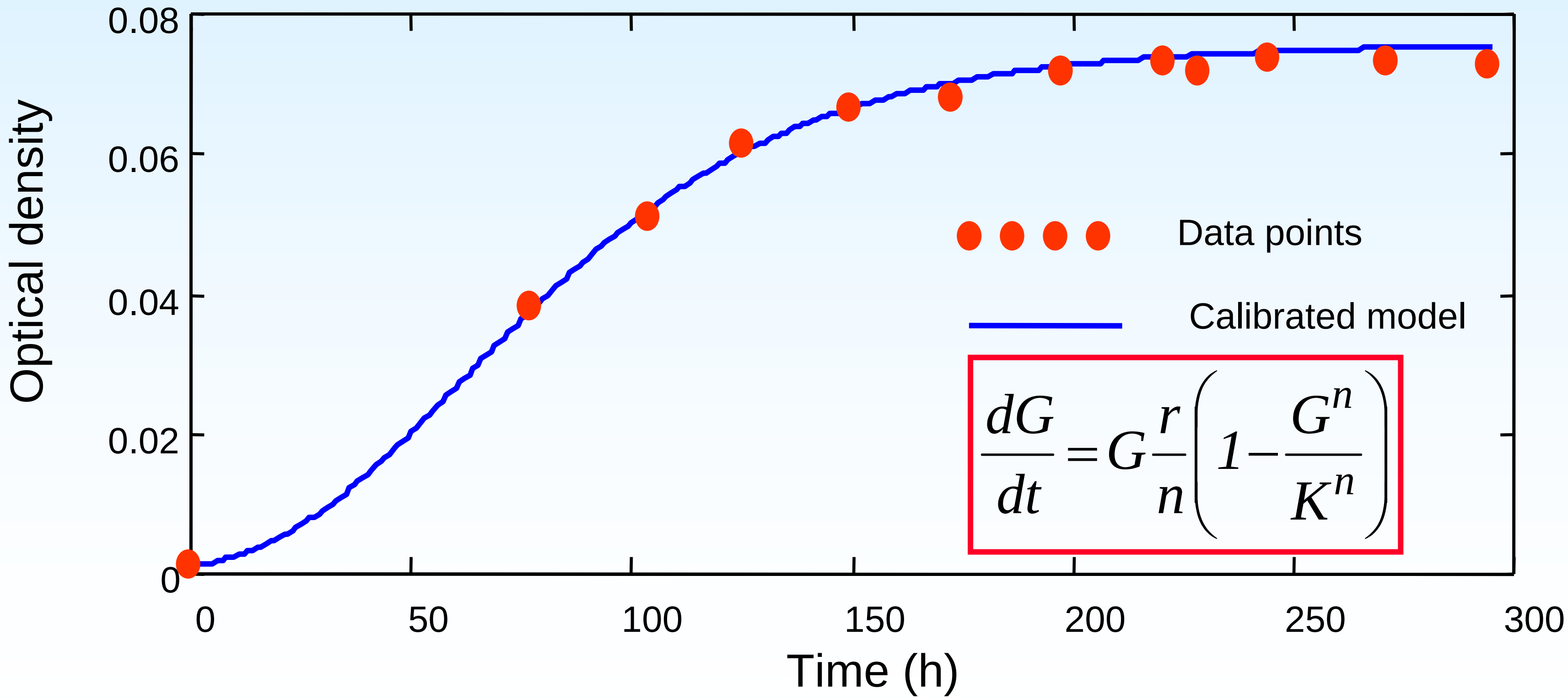


Case (2)



The Richards growth function

- Widely used in leaf and plant growth
- Saturation kinetics like the logistic, but with a further tuning parameter: the exponent *n*
- Model parameters calibrated on real experimental data *(Selenastrum algae)*



$$\frac{dG}{dt} = G\frac{r}{n}\left(1-\frac{G^n}{K^n}\right)$$

Parameter estimation

The simplex search was initiated from three different points

Not each choice terminated the search in the right place

Richards growth estimates from experimental data.

	r	*K*	*n*	Starting point	$E(\hat{\mathbf{p}})$
Case 1	0.02559	0.07530	0.05129	$[0.0239\ 0.08\ \ 0.05]^T$	1.40293 e-04
Case 2	0.01723	0.07793	-0.37804	$[0.090\ 0.095\ -0.65]^T$	2.04105 e-04
Case 3	0.02642	0.07459	0.08807	$[0.0800\ 0.09\ \ 0.15]^T$	2.04104 e-04

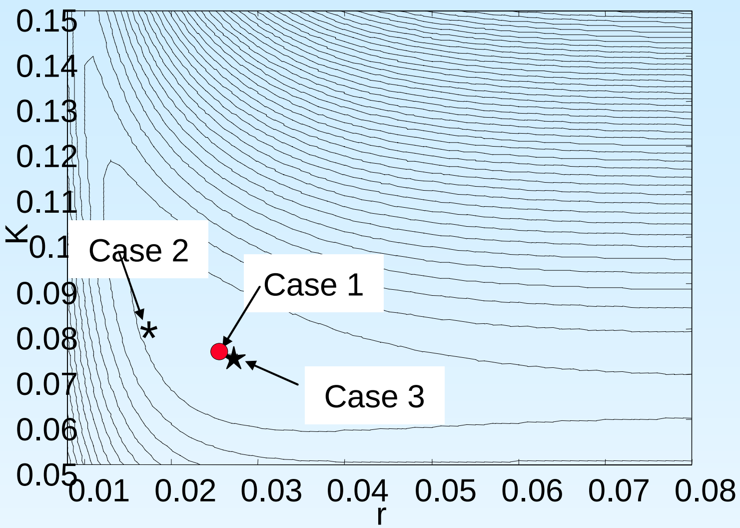
Case 1 estimated parameters

	r	*K*	*n*
Case 1	0.02559 ± 0.00445	0.07530 ± 0.00131	0.05129 ± 0.1947

Estimation problems with the Richards function

- The "true" parameters being not known, the ellipsoids method is the only way of assessing the reliability of the estimates.
- ***Case 1*** corresponds to a correct estimation: the search terminates in the minimum as confirmed by the exact coincidence of the Hessian and FIM ellipsoids. The intrinsic curvature correction factor has no effect.
- ***Case 2*** corresponds to a search termination at a point far from the minimum, where the gradient is still considerable
- ***Case 3*** represents the opposite situation: the search stopped in a flat region near, but not exactly at the minimum
- The exponent ***n*** is the most difficult parameter, with the possibility to obtain negative values.
- 95% confidence interval vary widely:
  - ***over 700% for n; less than 35% for r; only 3.5% for K***.

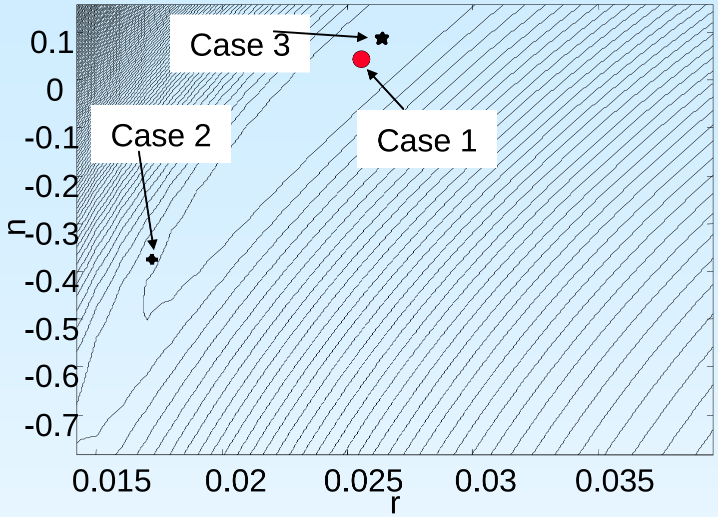
Location of search end-points

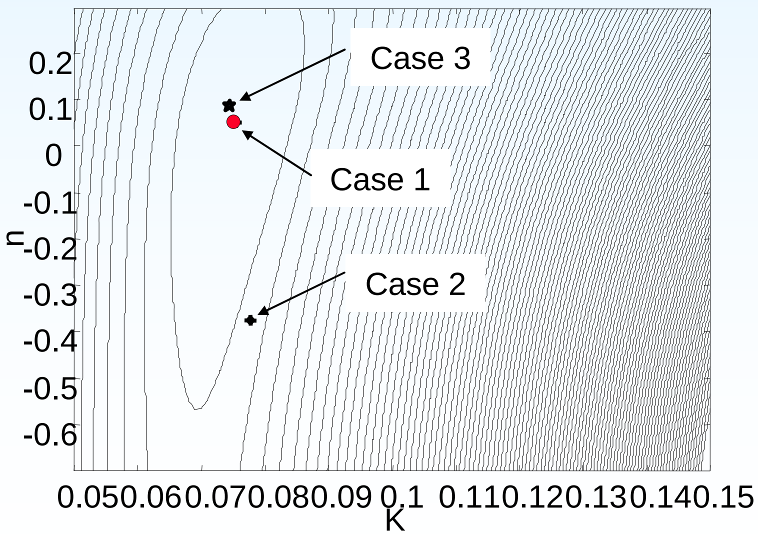


Only Case 1 reaches
the minimum.

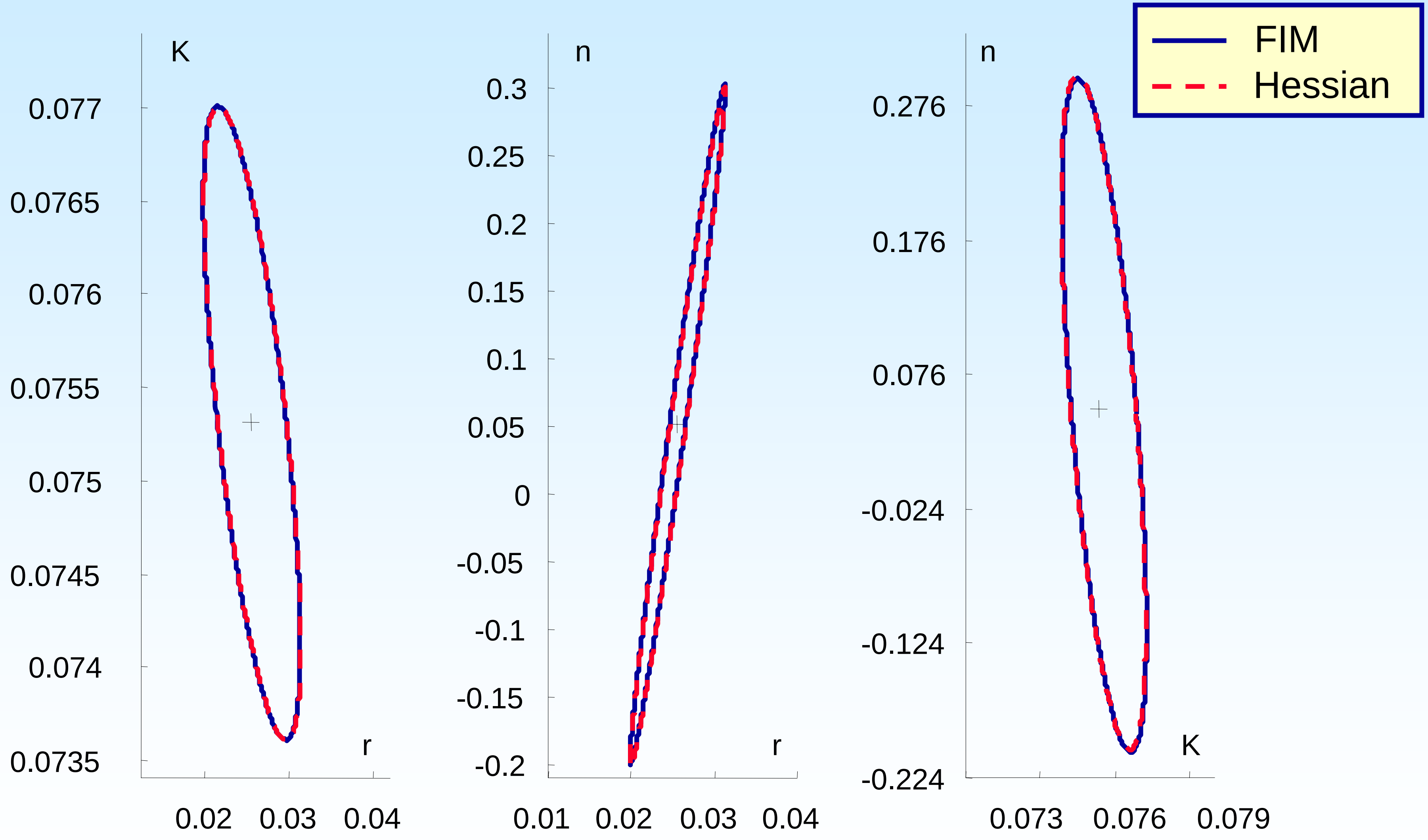
Case 2 in high gradient zone

Case 3 in flat region far from the minimum

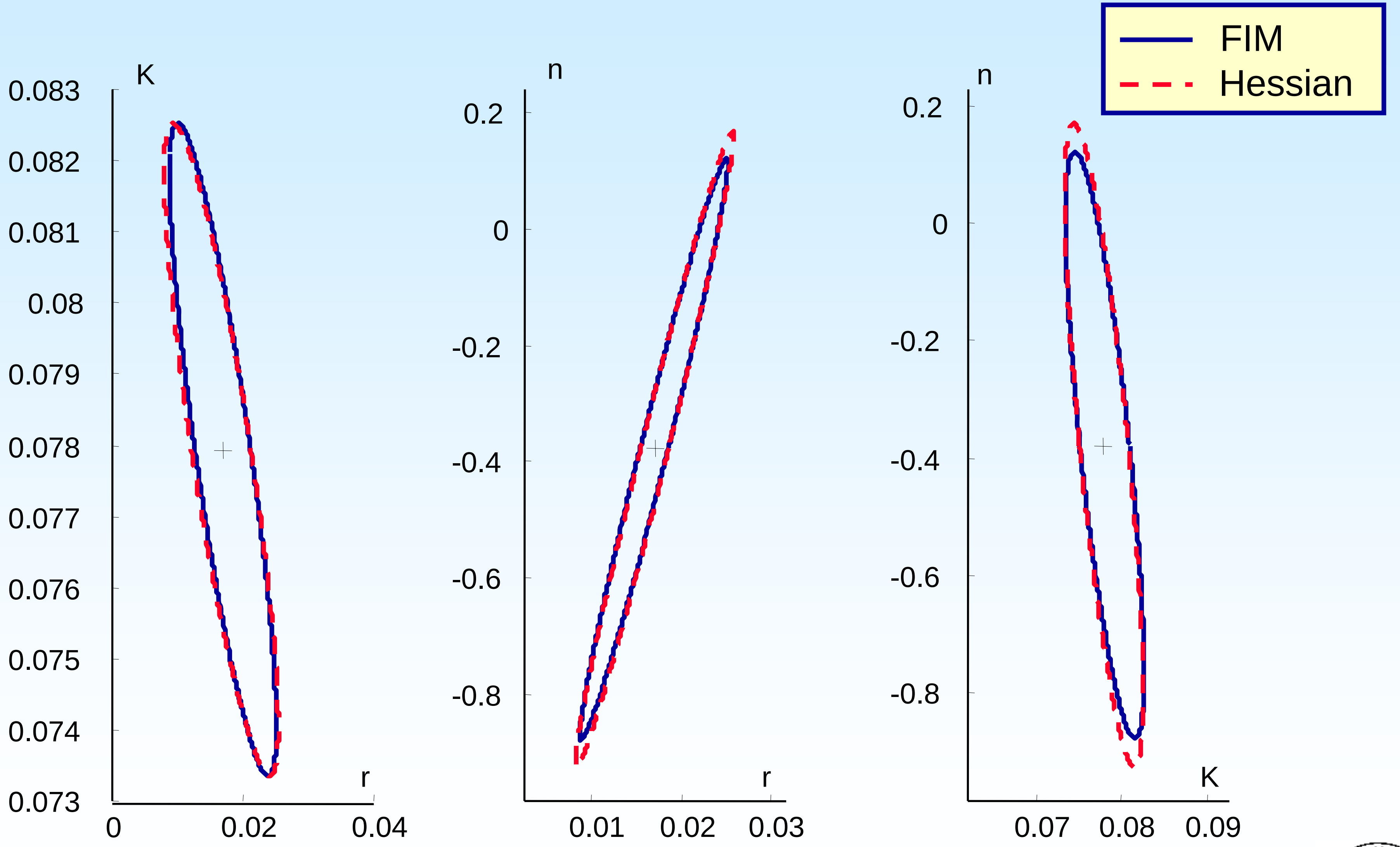




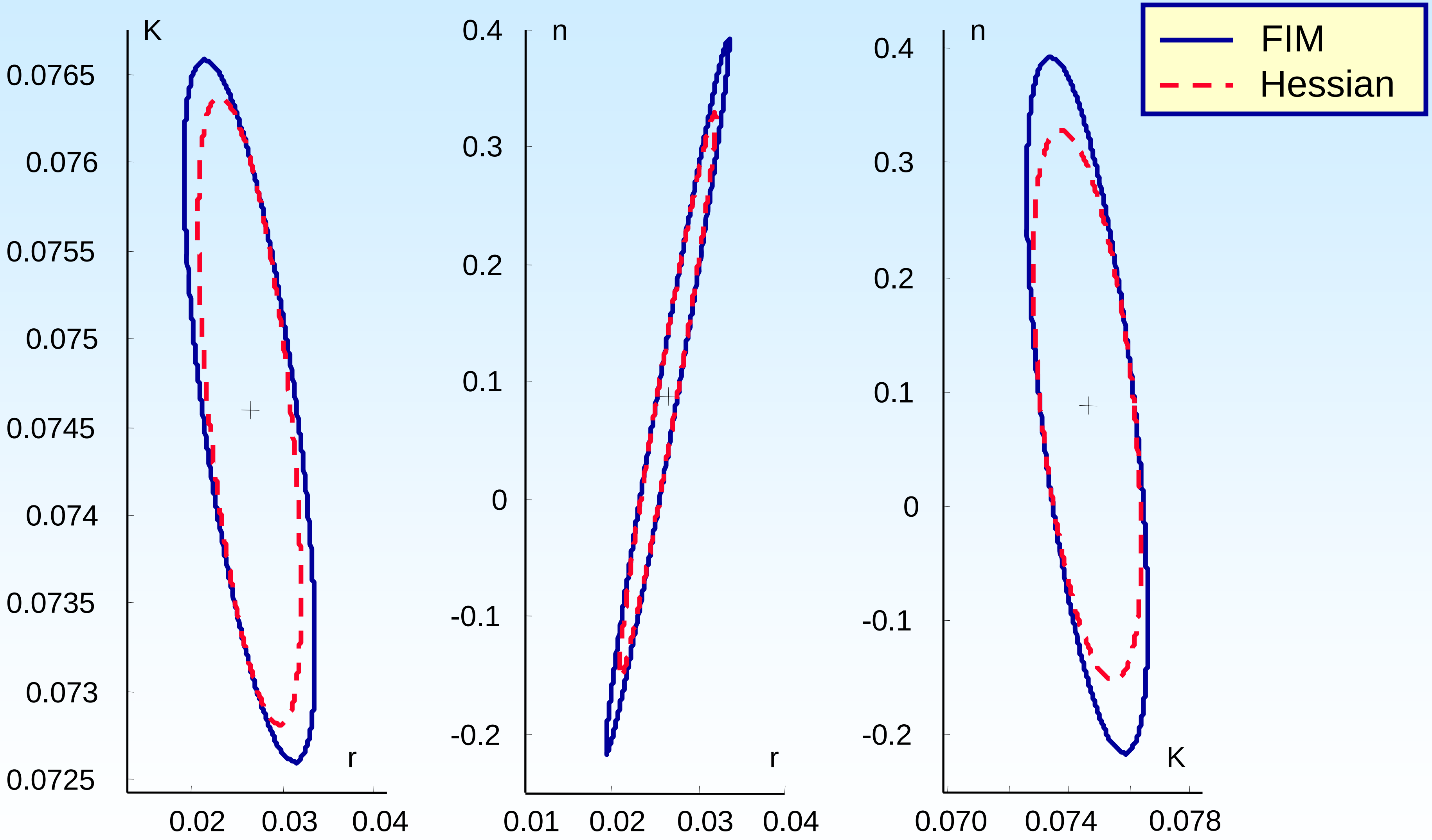
Case 1 Ellipsoids: coincidence



Case 2 Ellipsoids: Hessian larger than FIM



Case 3 Ellipsoids: FIM larger than Hessian

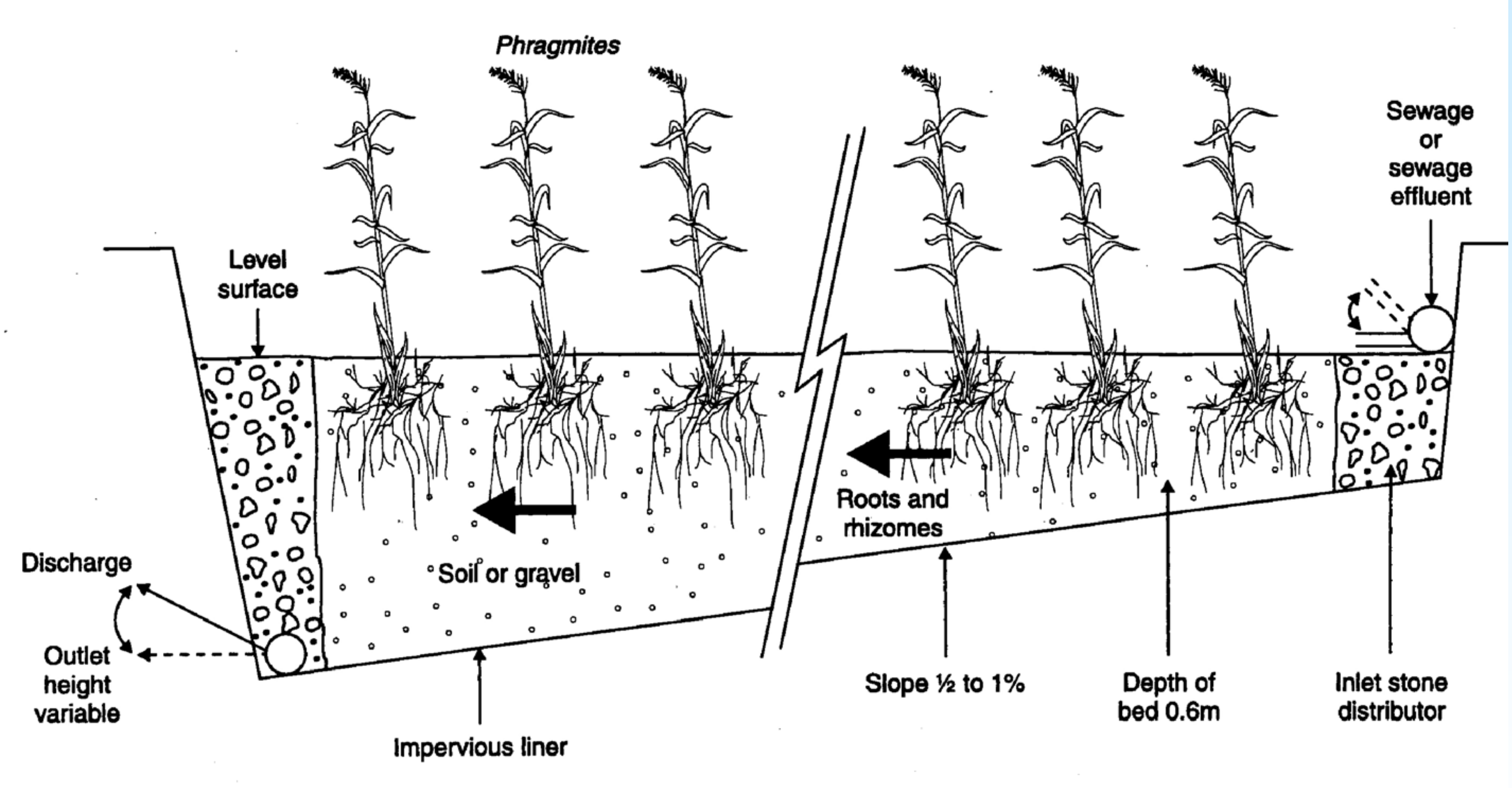


Application to dispersed flow

- Modelling the flow in Horizontal Subsurface Constructed Wetlands (HSCW)
- Flow behaviour is similar to a diffusive reactor (DR)
- If a DR is approximated with a combination of CSTR and Plug-Flow, the questions arise:
  - What is the best approximating structure?
  - How can we estimate its parameters?
- The theory is used here to answer both questions:
  - Propose a structure
  - Estimate the parameters

  - If the structure ***fails*** the confidence regions it is rejected
  - If the structure ***passes*** the confidence criterion it is **retained**
- Manuscript submitted to *Ecological Modelling*

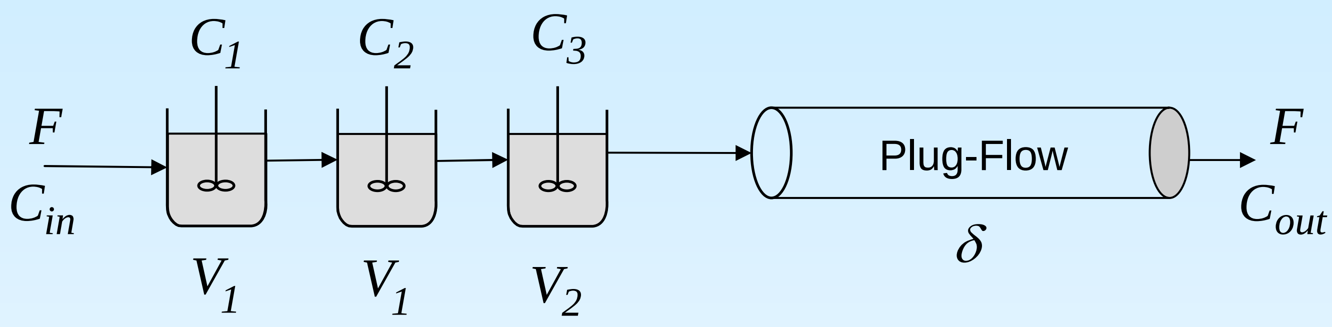
A typical HSCW



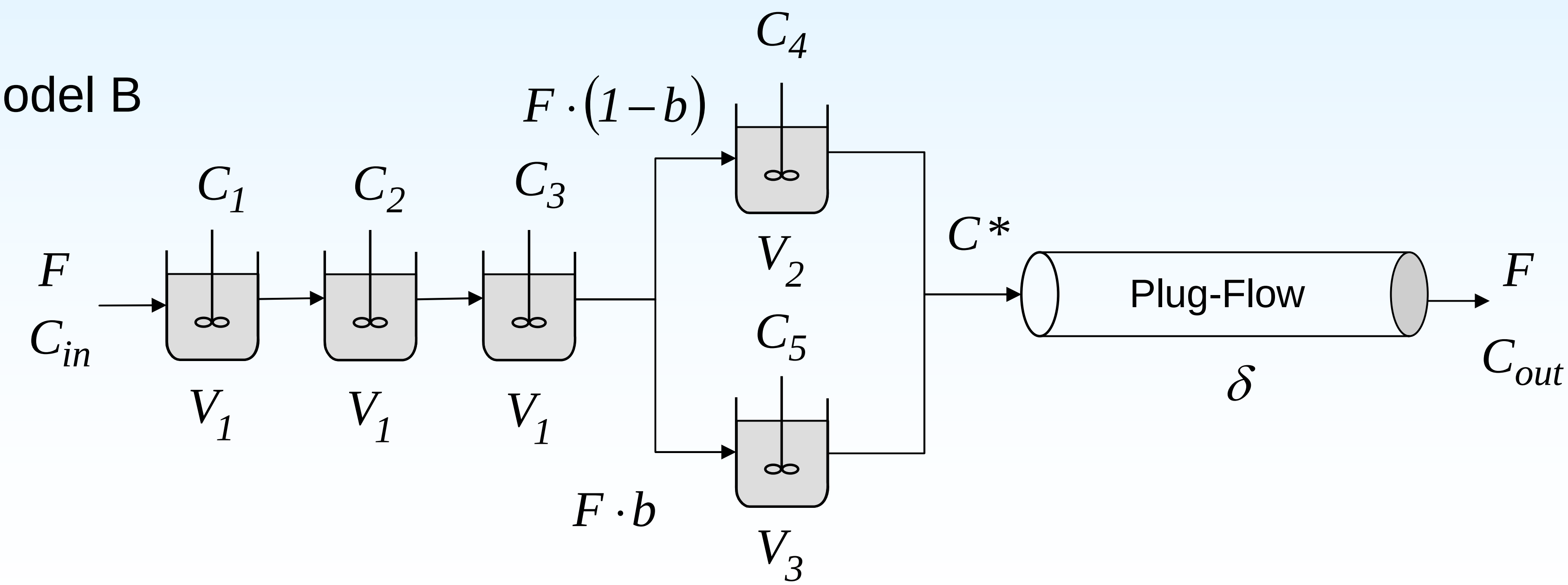
No reliable, simple flow model exists to date, which takes into account the variable porosity of the medium (gravel + roots)

Approximate structures

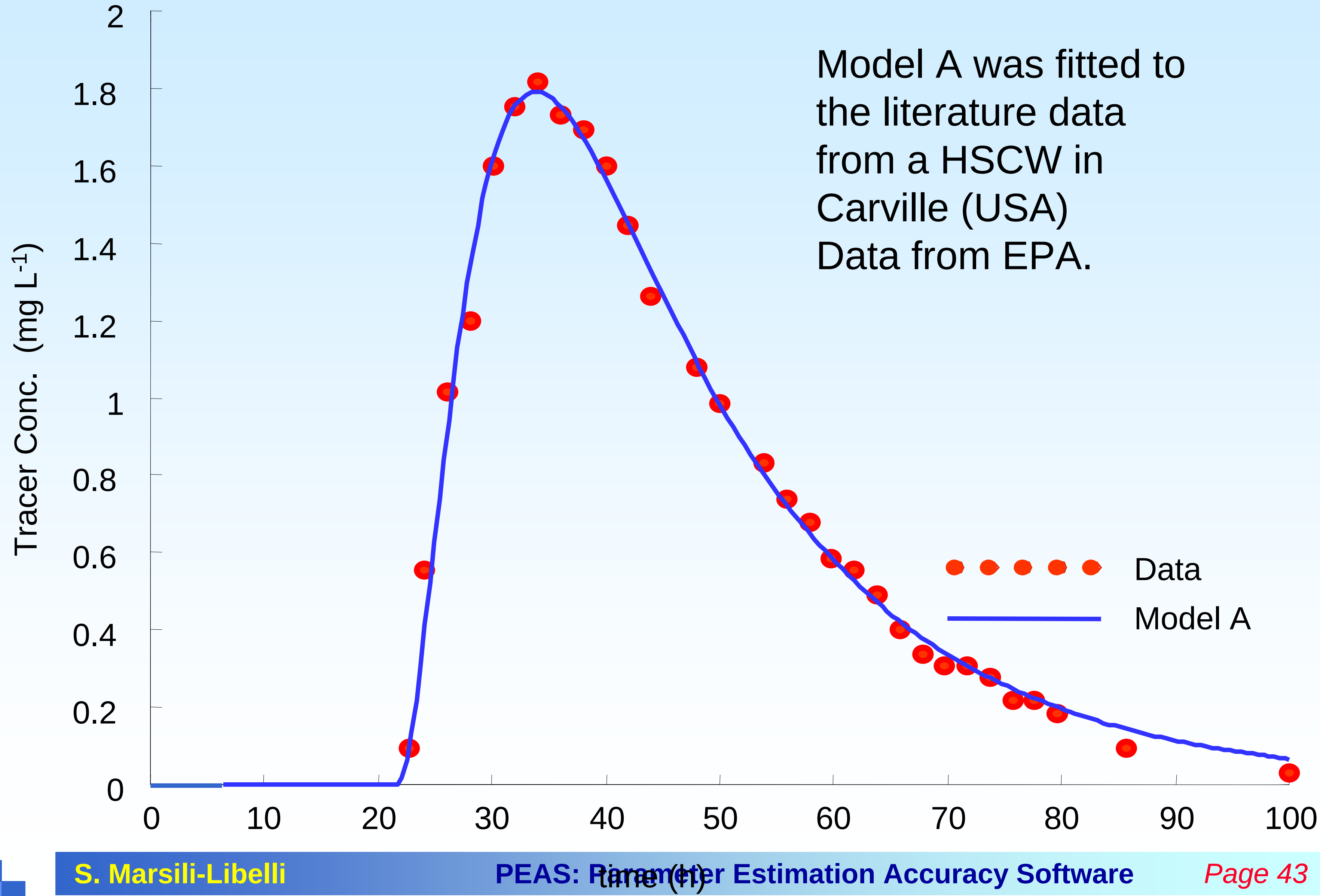
Model A



Model B

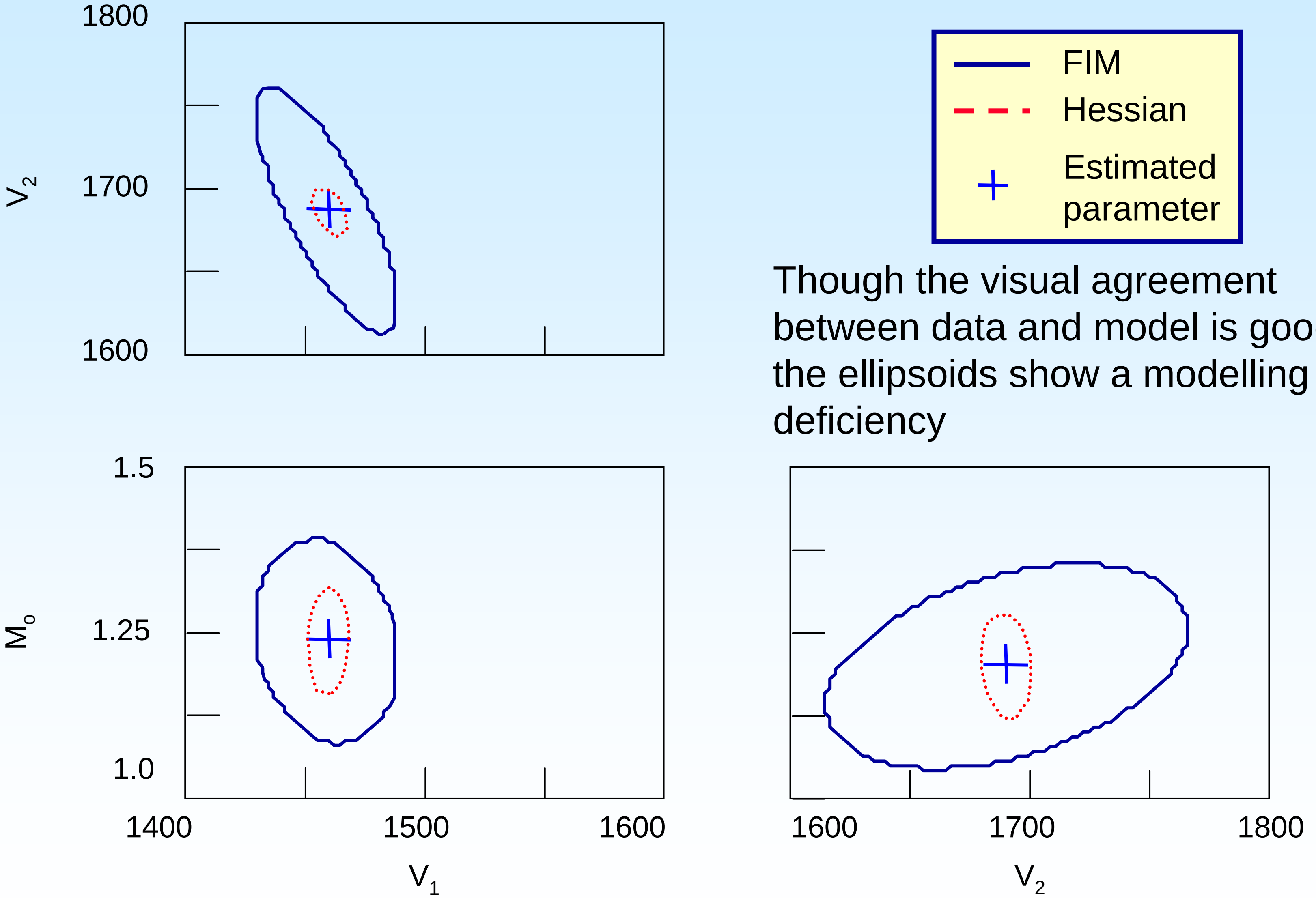


Model fitting: model A



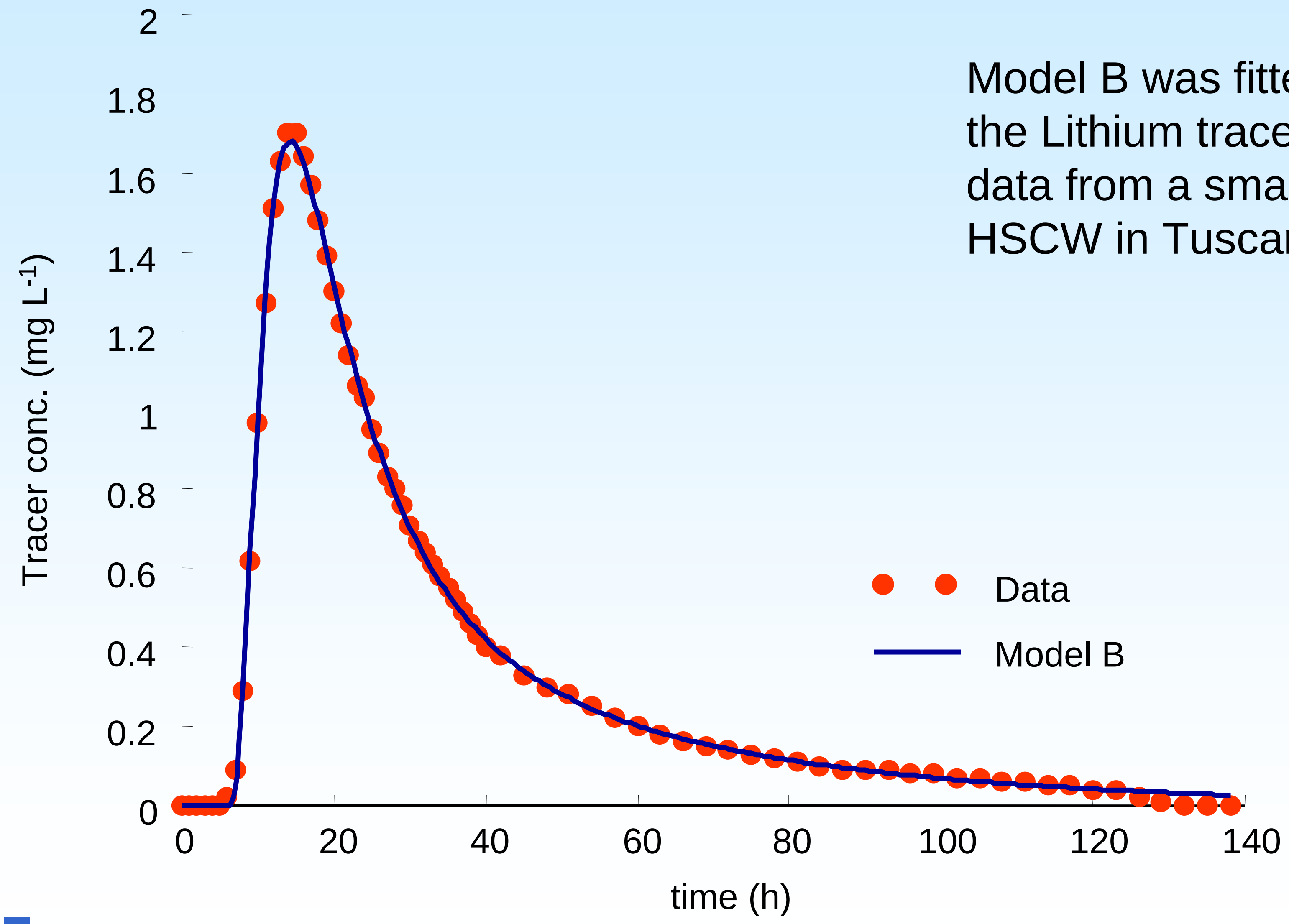
Model A was fitted to the literature data from a HSCW in Carville (USA) Data from EPA.

Assessment of model fitting: model A



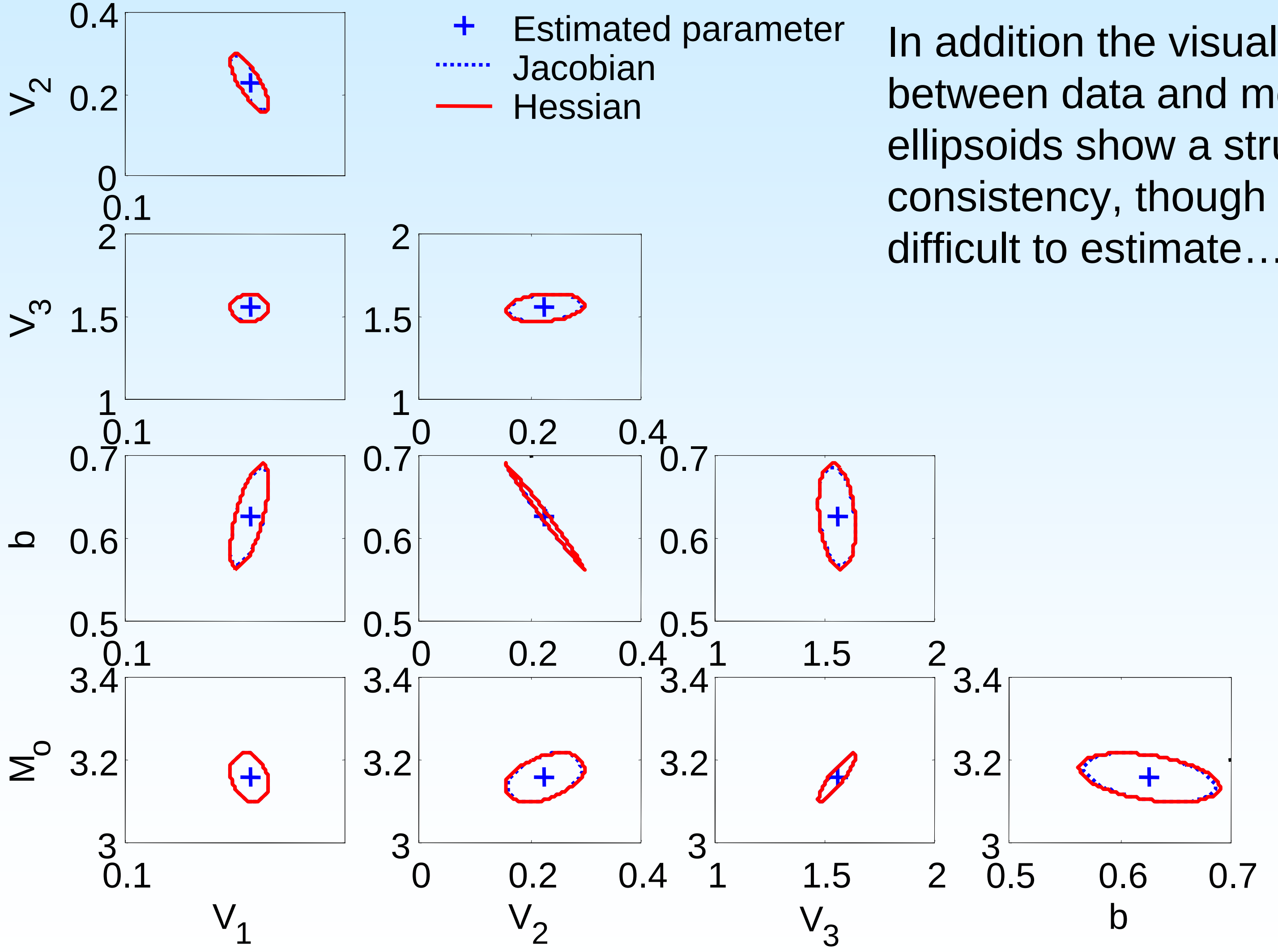
Though the visual agreement between data and model is good, the ellipsoids show a modelling deficiency

Model fitting: model B



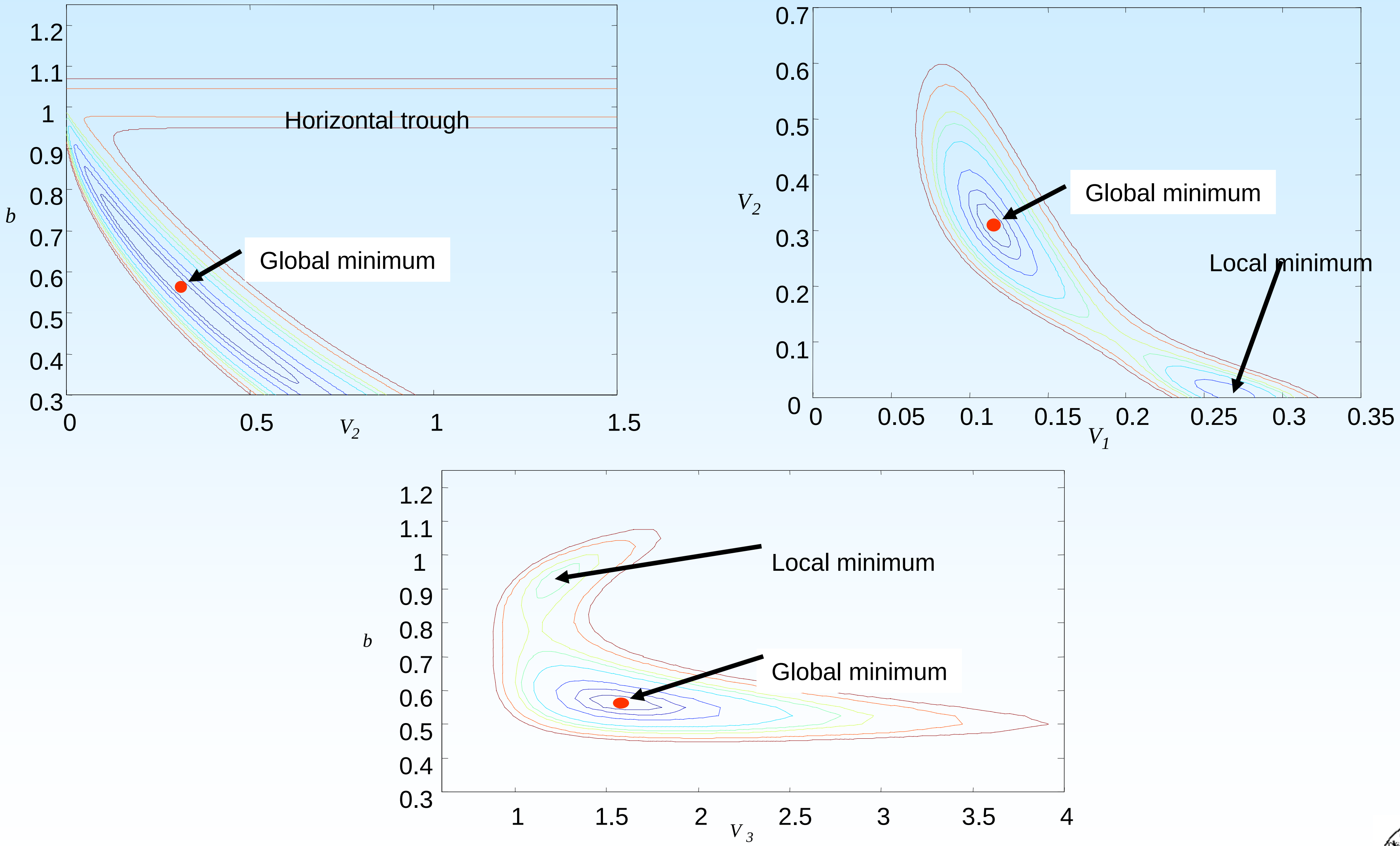
Model B was fitted to the Lithium tracer data from a small HSCW in Tuscany

Assessment of model fitting: model B

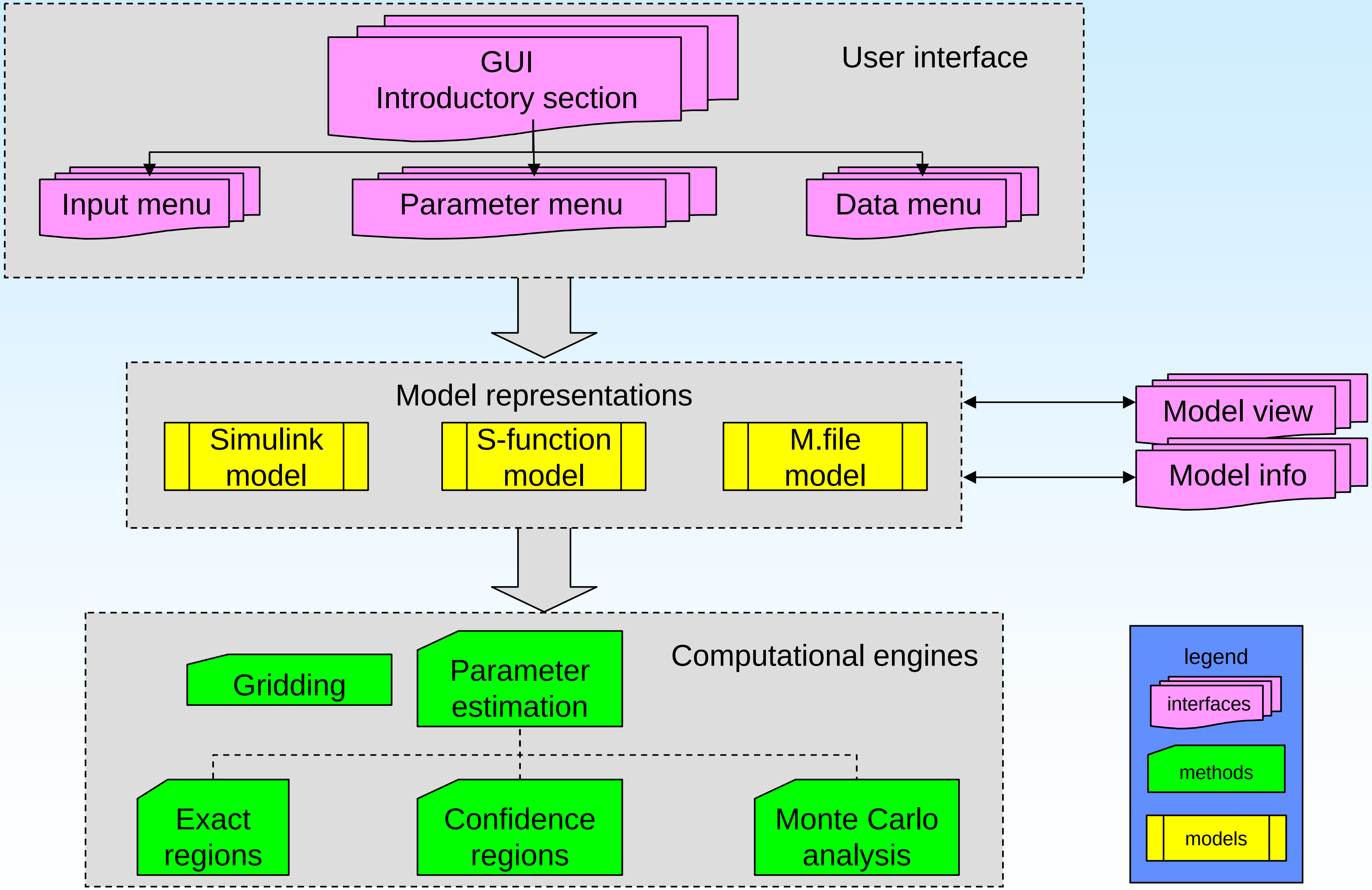


In addition the visual agreement between data and model, the ellipsoids show a structural consistency, though the model is difficult to estimate……..

Structural problems with model B



PEAS Structure



Software engineering

- Model definition
  - accepts model definitions
    - *.mdl
    - *.m
- Model specifications
  - model parameters (to be calibrated),
  - model constants (not to be calibrated)
  - initial conditions.
- Calibration specifications
  - choice of the optimization algorithm
  - estimation tolerances and termination criteria
- Accuracy assessment
  - exact regions
  - approximate regions
  - **Monte Carlo analysis**

Monte Carlo Analysis (MCA)

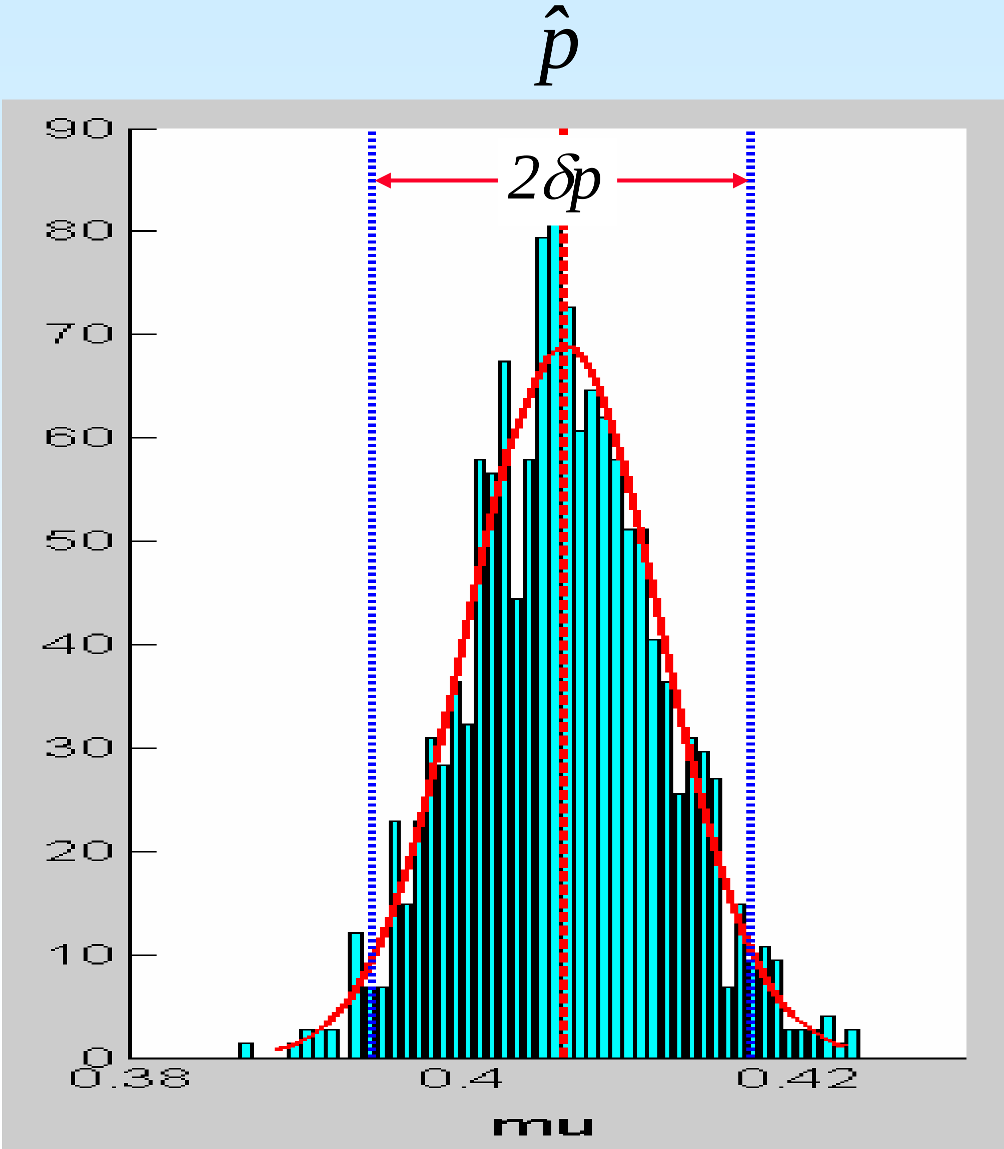
- There are cases in which the ellipsoid method is not applicable
  - e.g. in the case of “patched” models containing hard switching functions to introduce discontinuities in time-varying parameters
- With MCA the parameters confidence limits are obtained is based on a large number of estimations obtained by running the model with perturbed observations $\tilde{y} = y(\hat{\mathbf{p}}) \cdot (1+\varepsilon) \quad \varepsilon \in N(0,\sigma^2)$
- A gaussian distribution $N(\hat{m}_i, \hat{s}_i^2)$ is then fitted to the histogram of the estimates

$$\hat{p}_i \cong \hat{m}_i \; ; \delta p_i \cong \pm t_{N_{simul}-1}^{\alpha/2} \, \hat{s}_i$$

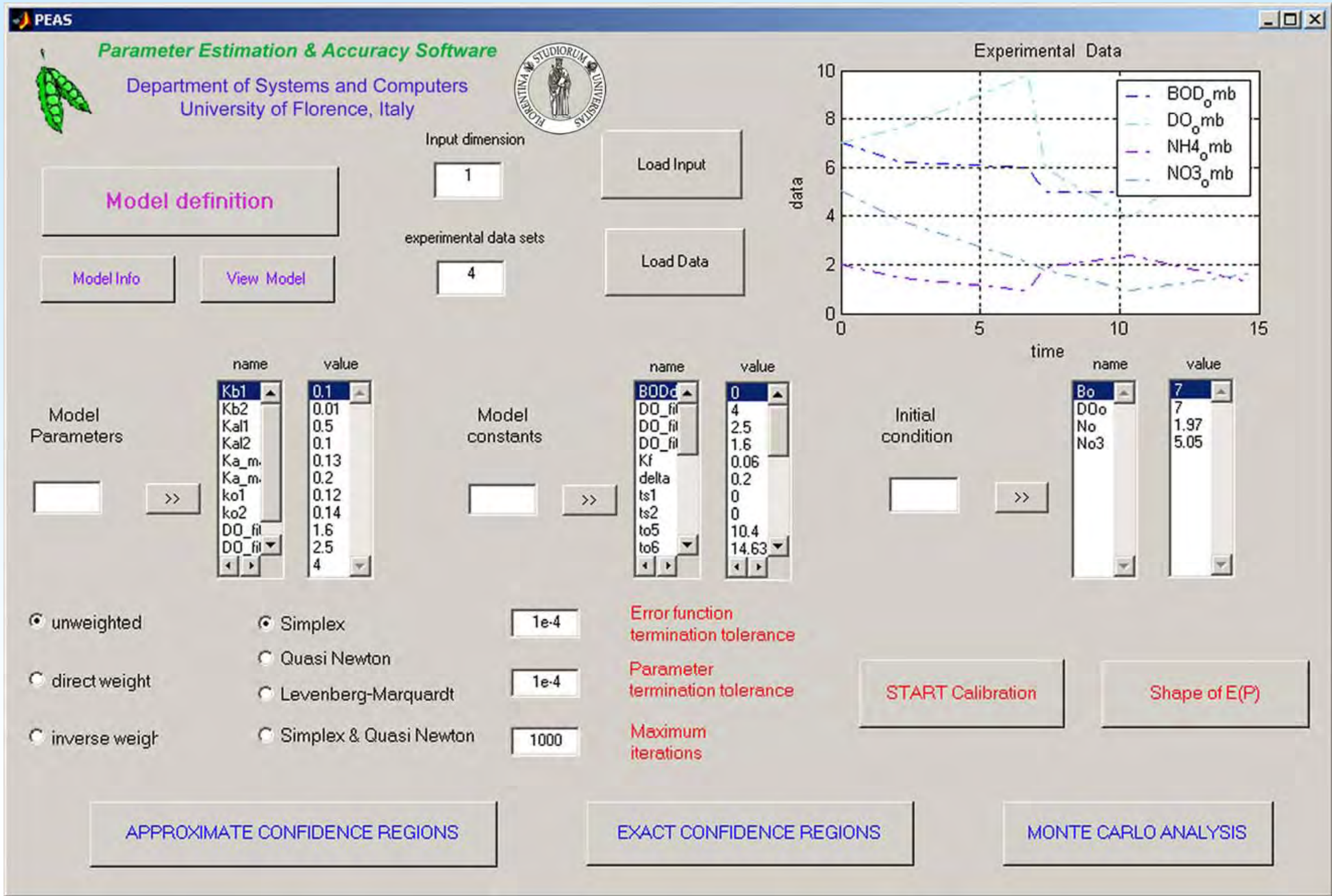
- with the variance approximated by

$$\hat{s}_i^2 = \frac{1}{N_{simul}-1} \sum_{j=1}^{N_{simul}} \left(p_j - \hat{m}_i\right)^2$$

Example of MCA results

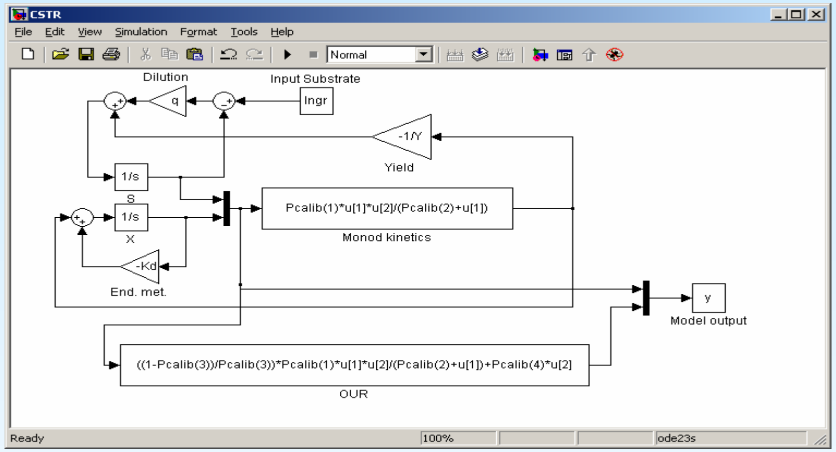


PEAS main interface

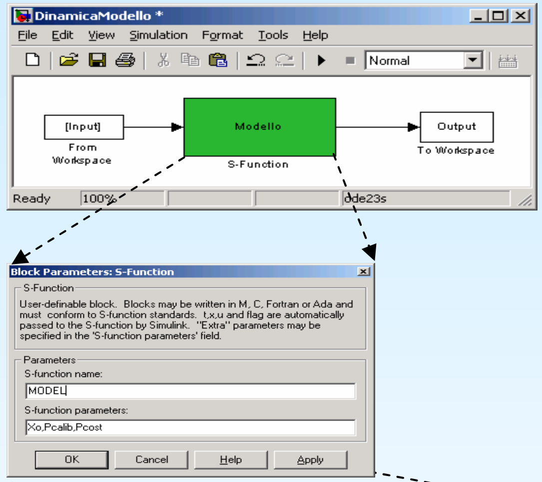


Model definition

Simulink model (block diagram)



Simulink model (S-function)



Simulink level

S-function level

```
#define S_FUNCTION_NAME MODEL
#define S_FUNCTION_LEVEL 2

#include "simstruc.h"
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
.........BODY of C source code
...................
#ifdef  MATLAB_MEX_FILE    /* Is this file
being compiled as a MEX-file? */
#include "simulink.c"      /* MEX-file
interface mechanism */
#else
#include "cg_sfun.h"       /* Code
generation registration function */
#endif
```

C level

↓

DLL

A dynamical model example

- A simple Monod model with respirometric observations

$$\frac{dS}{dt} = -\frac{1}{Y}\frac{mu\,S}{k_s + S}X + q(S_i - S)$$
$$\frac{dX}{dt} = \frac{mu\,S}{k_s + S}X - k_d X$$

$$r = \frac{1-Y}{Y}\frac{mu\,S}{k_s + S}X + k_d X$$

- In PEAS notation becomes

Model equations

$$\frac{dx_1}{dt} = -\frac{1}{P_{calib}(3)}\cdot P_{calib}(1)\cdot x_1 \cdot \frac{x_2}{P_{calib}(2) + x_1} + P_{cost}(1)\cdot(Input - x_1)$$
$$\frac{dx_2}{dt} = P_{calib}(1)\cdot x_1 \cdot \frac{x_2}{P_{calib}(2) + x_1} - P_{calib}(4)\cdot x_2$$

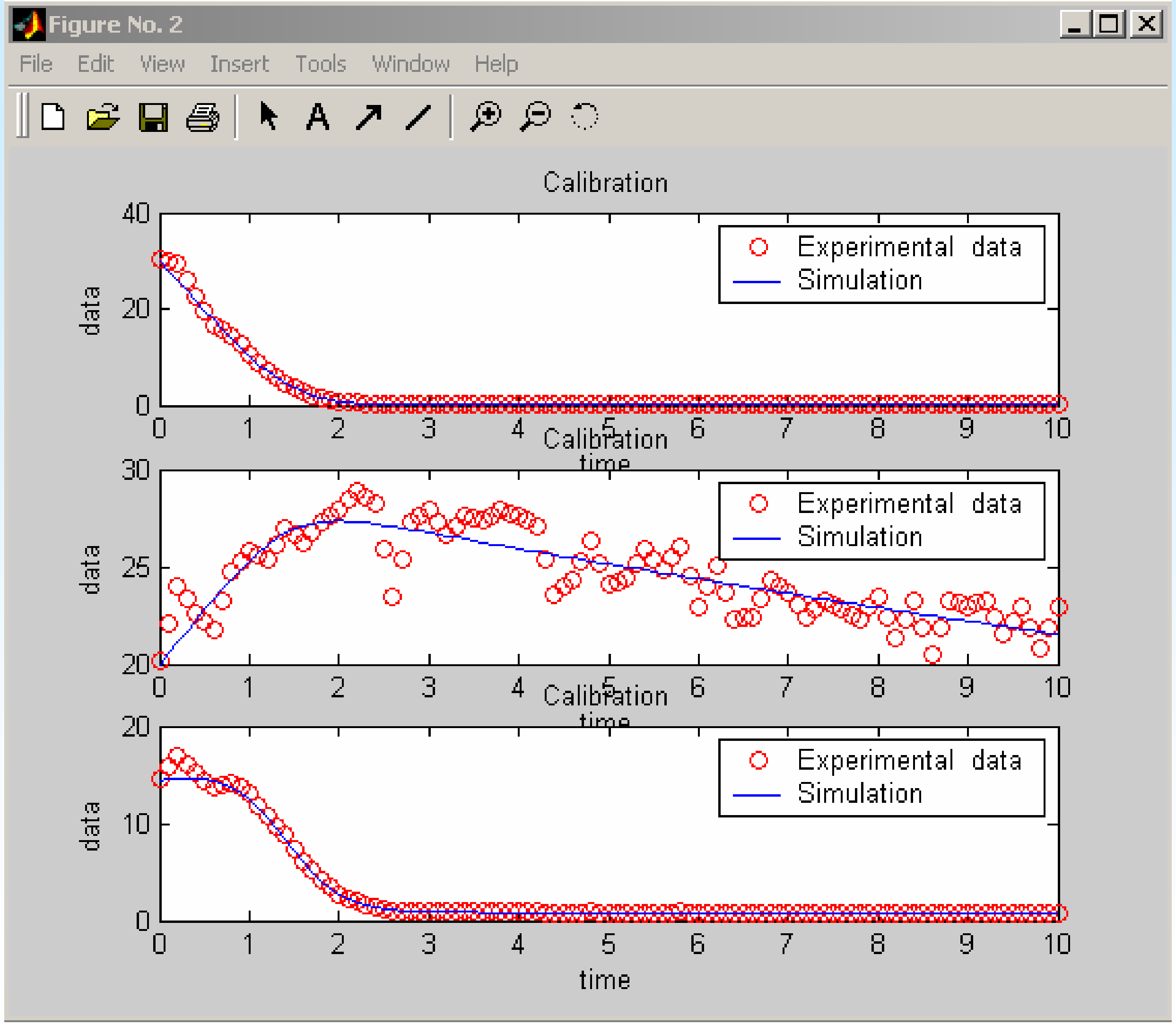
Output equations

$$y_1 = x_1$$
$$y_2 = x_2$$
$$y_3 = \frac{1 - P_{calib}(3)}{P_{calib}(3)}\cdot\frac{P_{calib}(1)\cdot x_1 \cdot x_2}{P_{calib}(2) + x_1} + P_{calib}(4)\cdot x_2$$

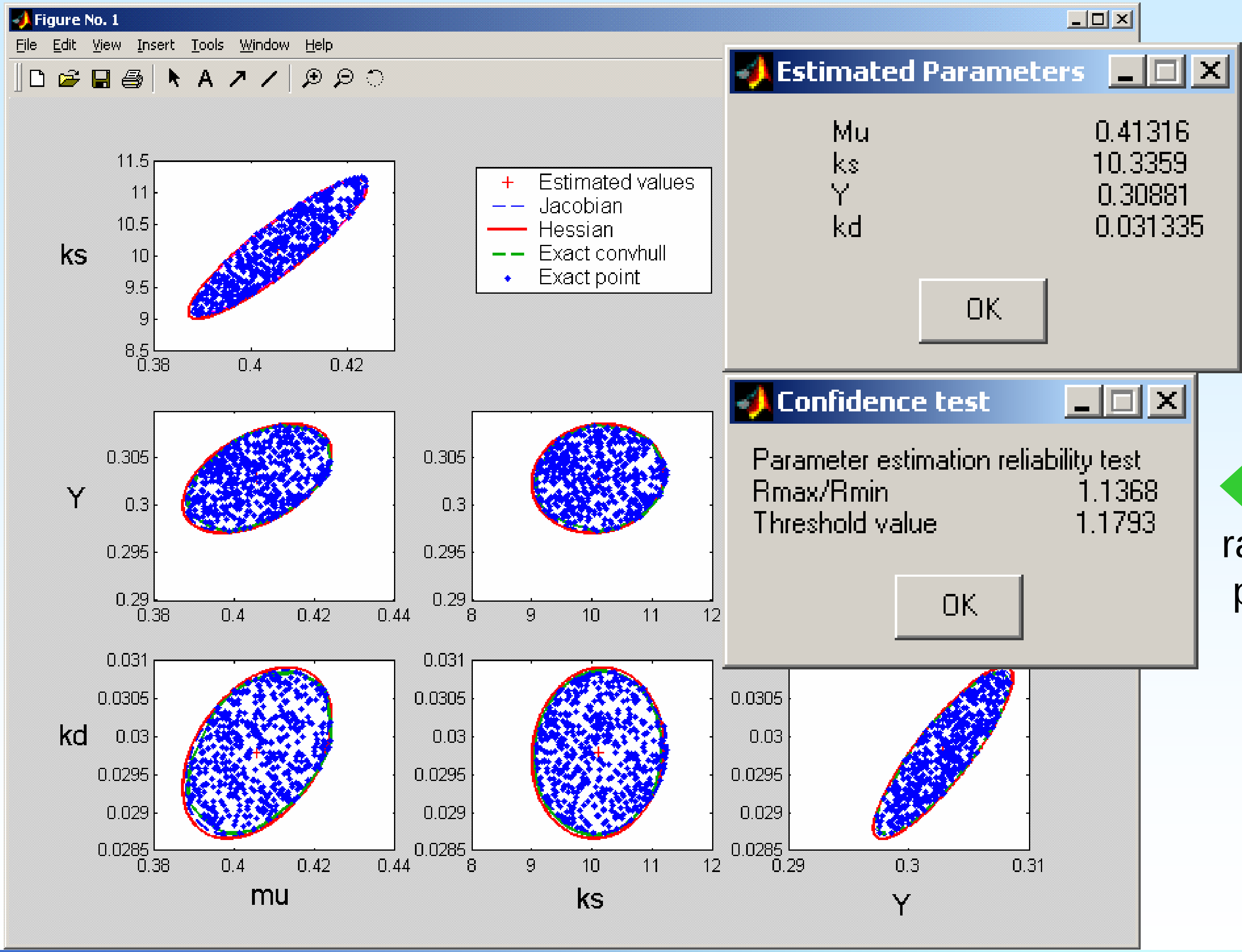
Error functional

$$E(\boldsymbol{p}) = \sum_{j=1}^{N}\left(y_1^{exp}(j) - y_1(j)\right)^2 + \sum_{j=1}^{N}\left(y_2^{exp}(j) - y_2(j)\right)^2 + \sum_{j=1}^{N}\left(y_3^{exp}(j) - y_3(j)\right)^2$$

Calibration results

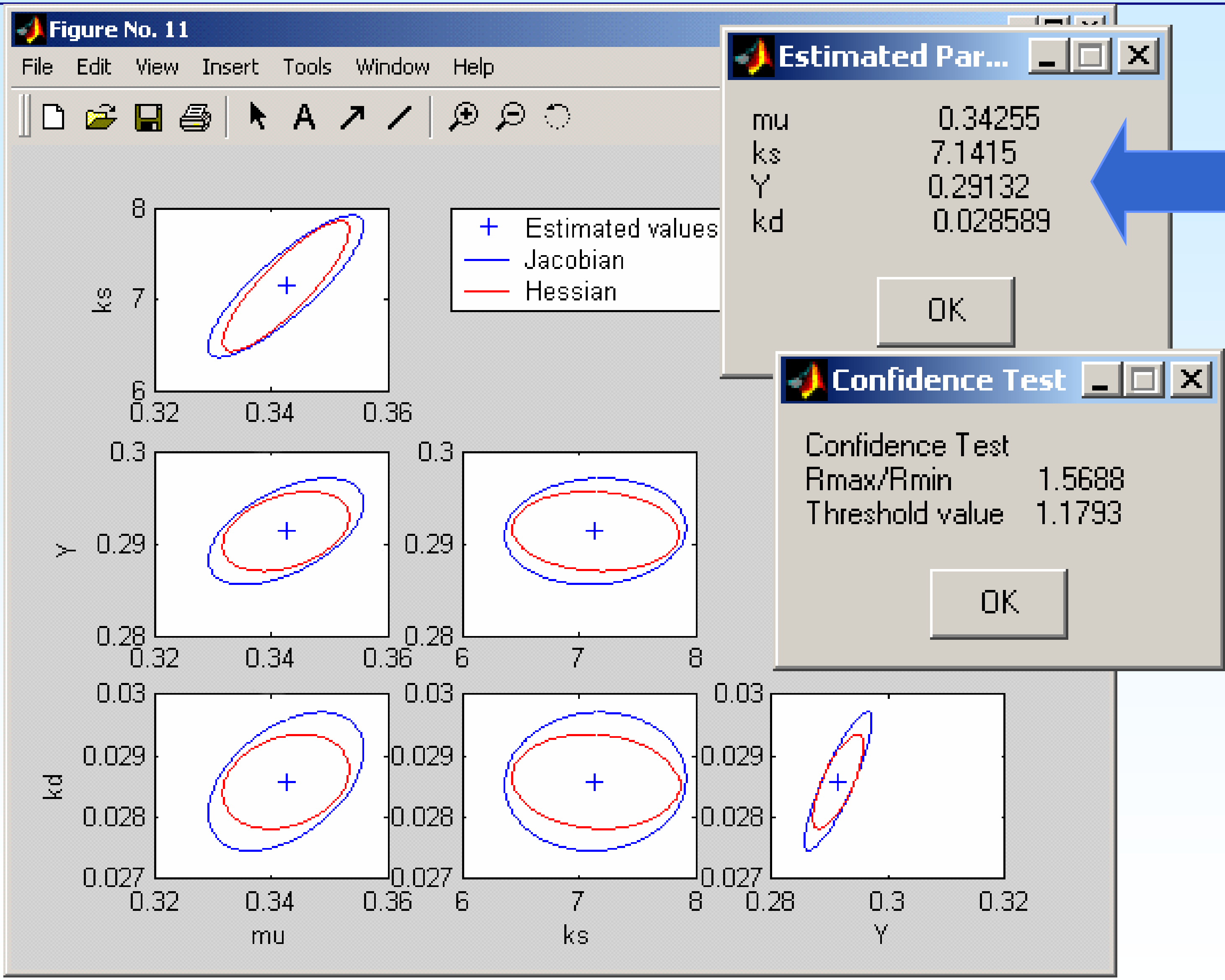


Confidence regions



radii test passed

Bad result due to improper initialization



"good" estimates

0.41316
10.3359
0.30881
0.031335

radii test failed

Comparison of algorithmic performance

The Simplex method is the most accurate and, in this case, the application of the Quasi-Newton method brings no improvement. The other algorithms are faster but produce less accurate results

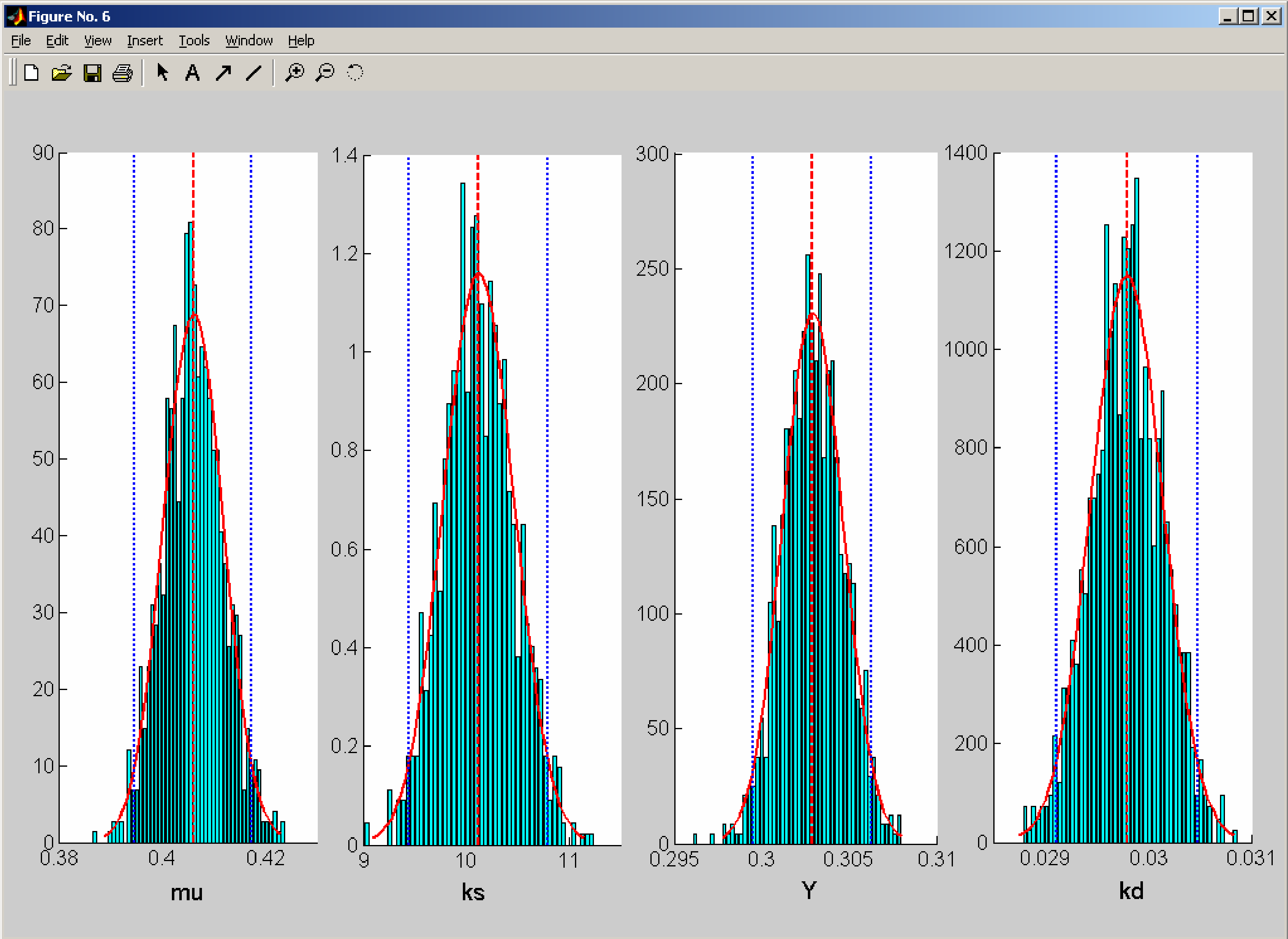
Parameter	True value	Initial value	Optimization algorithm			
			Simplex	Quasi-Newton	Levemberg Marquardt	Simplex + Quasi-Newton
mu	0.4	0.3	0.4055	0.42432	0.43548	0.4055
ks	10	12	10.1022	11.3514	12.0871	10.1022
Y	0.3	0.2	0.3029	0.30337	0.3037	0.3029
kd	0.03	0.04	0.0298	0.02985	0.02991	0.0298
run time (s)			63.703	83.015	10.25	146.734
E(p)			16.1021	16.7196	17.5577	16.1021

Confidence interval comparison

confidence bounds obtained with the approximate confidence regions based on the Hessian matrix approximation and with the Monte Carlo analysis for an estimated measurement error $s^2 = 0.05$.

Parameter	True value	Estimated value	
		Simplex (Hessian)	Monte Carlo
mu	0.4	0.40552 ± 0.0120	0.40593 ± 0.01135
ks	10.0	10.1022 ± 0.7097	10.1235 ± 0.67438
Y	0.3	0.30287 ± 0.0037	0.30293 ± 0.003392
kd	0.03	0.02979 ± 0.0007	0.029795 ± 0.00068

Monte Carlo analysis



An algebraic model

- The oxygen dynamics $\frac{dS_o}{dt} = K_L a(S_{sat} - S_o) - r$
- and its analytical solution obtained by calculus

$$S(t) = S_{sat} \cdot \left(1 - e^{-K_L a \cdot t}\right) + S_o(0) \cdot e^{-K_L a \cdot t} - \frac{r}{K_L a} \cdot \left(1 - e^{-K_L a \cdot t}\right)$$

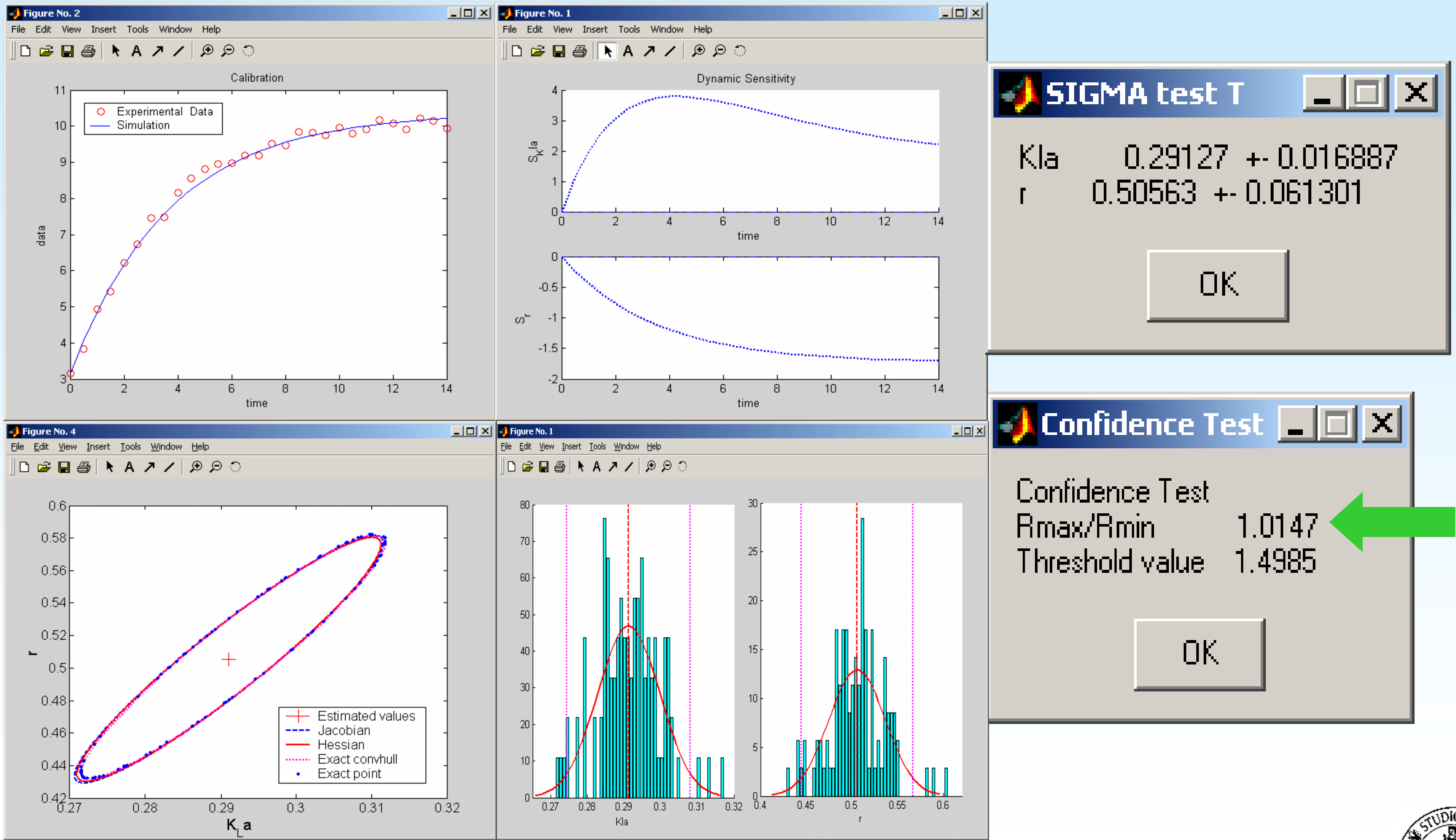
- PEAS notations $P_{calib}(1) = K_L a;\ P_{calib}(2) = r;\ P_{cost}(1) = S_{sat};\ X_o(1) = S_o$

yield $S = P_{cost}(1) \cdot \left(1 - e^{-P_{calib}(1)t}\right) + X_o \cdot e^{-P_{calib}(1)t} - \frac{P_{calib}(2)}{P_{calib}(1)} \cdot \left(1 - e^{-P_{calib}(1)t}\right)$

- Coded as an m. file

```
function [S,tsim]=Rear(t)
global P_calib P_cost X_0 Input Q
S=(P_cost(1)).*(1-exp(-P_calib(1).*(t)))+…
(X_0(1).*exp(-P_calib(1).*(t)))-…
(P_calib(2)./P_calib(1)).*(1-exp(-P_calib(1).*(t)));
tsim=t;
```

Algebraic model calibration results



Conclusions

- ***Confidence regions*** provide a way to assess estimation ***consistency***
- Two differing approximations can be used:
  - ***FIM*** involving model linearisation and sensitivity analysis
  - ***Hessian***, based on a second order approximation of the error functional
  - Their difference involves *curvature*
- PEAS implements both the estimation AND the accuracy analysis
  - Both exact and approximate confidence regions can be computed
- A numerical "pass" test based on curvature radii is included
- If the ellipsoids method is not applicable, Monte Carlo analysis is available


"That's all Folks!"