UNIVERSITEIT GENT

FACULTY OF ENGINEERING AND ARCHITECTURE

Effect of error propagation in successive parameter estimation

V. Kumar[1], *N. Kerimoglu*[2], *J.W. Thybaut*[1], *A. Mhamdi*[2], *G.B. Marin*[1] *and W. Marquardt*[2]

[1] Laboratory of Chemical Technology, Ghent University, Ghent, 9000, Belgium
[2] AVT-Process Systems Engineering, RWTH Aachen University, Aachen, 52056, Germany

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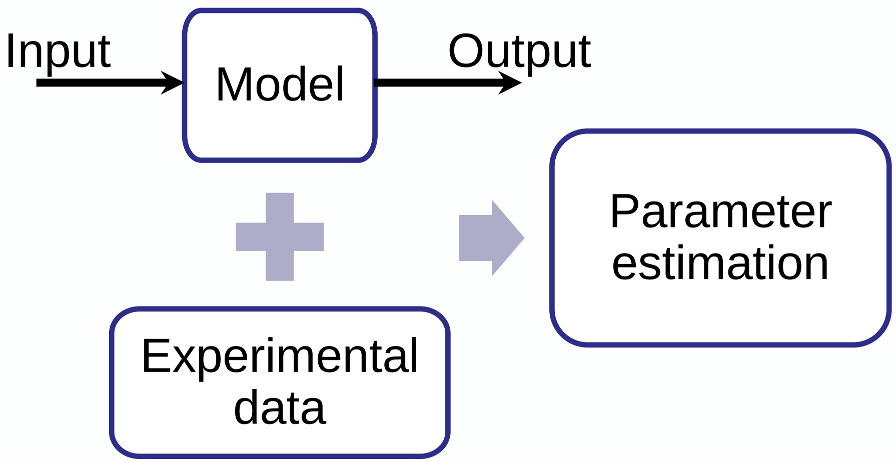
introduction

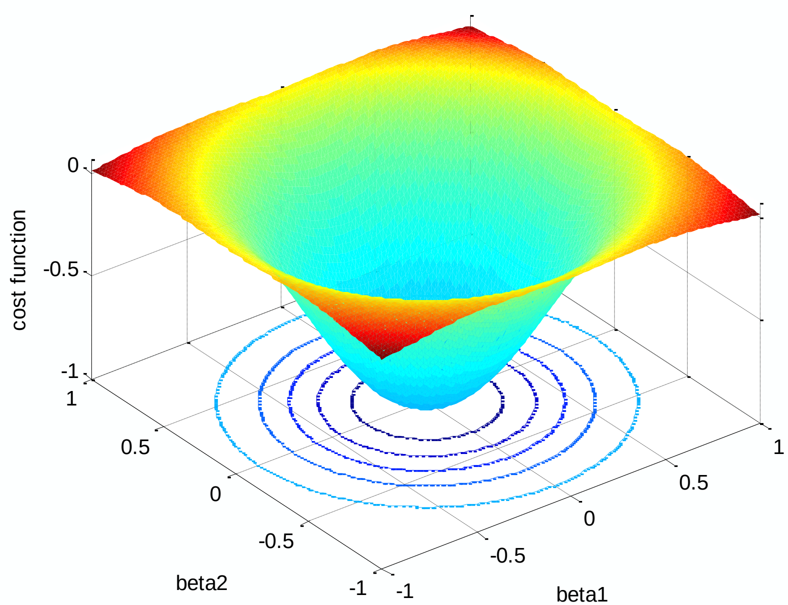


Physical meaning

- Scientific background
- Experimental details

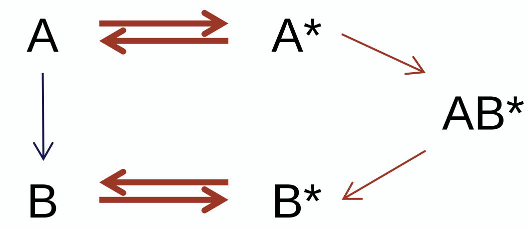
Mathematical representation

- Model complexity
- Convergence

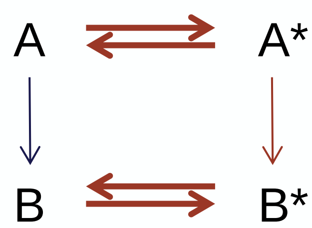


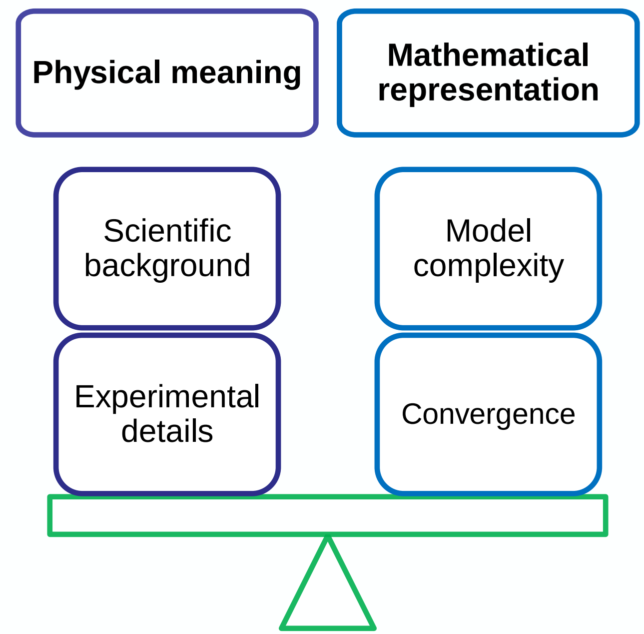
balancing the "pillars"

- Ill-conditioning of the system
  - Identifiability of parameters



- How?
  - Reduce complexity
  - Fix parameters
    - A-priori determined
    - Literature





objective

- Uncertainty in the determined parameter(s) **not accounted**
  - Measurements errors
  - Theoretical calculations

To study the propagation of error in the fixed parameters in successive parameter estimation

outline

- Introduction
- Mathematical background
  - Linear regression analysis
- Case study
  - Well-conditioned
  - Ill-conditioned
  - Reaction kinetics example
- Conclusions

linear regression analysis

All parameters estimated

$$\tilde{Y} = X\beta + \xi \qquad \xi = N\left(0, V(\xi)\right)$$

$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}}\left[\left(\tilde{Y} - X\beta\right)^{2}\right]$$

using linear transformations;

$$\hat{\beta} = \left(X^{T}X\right)^{-1}X^{T}\tilde{Y}$$

$$\hat{\beta} = \beta + \varepsilon \qquad \varepsilon = N\left(0, V(\varepsilon)\right)$$

$\hat{\beta}$ is the true estimate of β with an error, $\boldsymbol{\varepsilon}$

(Nomenclatures as in Neter, J., et al. (1996). Applied Linear Statistical Models)

linear regression analysis

$$\hat{\beta} = \left(X^T X\right)^{-1} X^T \tilde{Y}$$

$$V\left(\hat{\beta}\right) = \left(X^T X\right)^{-1} X^T V(\xi) X^T \left(X^T X\right)^{-1}$$

Mathematically,

$$B = AY$$

$$V(B) = V(AY)$$

$$V(B) = AV(Y)A^T$$

In case of constant variance in the measurement error

$$V(\xi) = I\sigma^2$$

by applying matrix operations to the above equation;

$$V\left(\hat{\beta}\right) = \left(X^T X\right)^{-1} \sigma^2$$

linear regression analysis

A subset of parameters is fixed

$$\tilde{Y} = X_1\beta_1 + X_2\beta_2 + \xi$$

$$\hat{\beta}_1 = \beta_1 + \delta \qquad \delta = N\left(0, V(\delta)\right)$$

$$\hat{\beta}_2 = \underset{\beta_2}{\operatorname{argmin}}\left[\left(\left(\tilde{Y} - X_1\beta_1\right) - X_2\beta_2\right)^2\right]$$

using linear transformations;

$$\hat{\beta}_2 = \left(X_2^T X_2\right)^{-1} X_2^T\left(\tilde{Y} - X_1^T\beta_1\right)$$

$$\hat{\beta}_2 = \beta_2 + \varepsilon \qquad \varepsilon = N\left(0, V(\varepsilon)\right)$$

Propagation of variances measurement error and Variances in fixed parameters into the estimated parameters

$$V(\hat{\beta}_2) = \left(X_2{}^T X_2\right)^{-1} X_2{}^T\left[V(\tilde{Y} - X_1^T\beta_1)\right]X_2\left(X_2{}^T X_2\right)^{-1}$$

linear regression analysis

Variances of the modified measurements,

$$V(\tilde{Y} - X_1^T \beta_1) = V(\tilde{Y}) - 2\,\mathrm{cov}(\tilde{Y}, X_1^T \beta_1) + X_1 V(\beta_1) X_1^T$$

Replacing above expression in the expression for $V(\hat{\beta}_2)$

$$V(\hat{\beta}_2) = \left(X_2^{\,T} X_2\right)^{-1} X_2^{\,T} \left[V(\tilde{Y} - X_1^T \beta_1)\right] X_2 \left(X_2^{\,T} X_2\right)^{-1}$$

$$V(\hat{\beta}_2) = \left(X_2^{\,T} X_2\right)^{-1} X_2^{\,T} \left[V(\tilde{Y}) - 2\,\mathrm{cov}(\tilde{Y}, X_1^T \beta_1) + X_1 V(\beta_1) X_1^{\,T}\right] X_2 \left(X_2^{\,T} X_2\right)^{-1}$$

Writing $V(\hat{\beta}_2)$ in terms of errors,

$$V(\hat{\beta}_2) = \left(X_2^{\,T} X_2\right)^{-1} X_2^{\,T} \left[V(\xi) - \cancel{2\,\mathrm{cov}(\xi, X_1^T \delta)} + X_1 V(\delta) X_1^{\,T}\right] X_2 \left(X_2^{\,T} X_2\right)^{-1}$$

No correlation between the error in measurements and the error in fixed parameter(s)

$$\Rightarrow \quad V(\hat{\beta}_2) = \left(X_2^{\,T} X_2\right)^{-1} X_2^{\,T} \left[V(\xi) + X_1 V(\delta) X_1^{\,T}\right] X_2 \left(X_2^{\,T} X_2\right)^{-1}$$

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  - Ill-conditioned
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well versus ill conditioned systems

$$\tilde{Y} = X_1\beta_1 + X_2\beta_2 + \xi$$

System 1

$$X_1 = [3 \quad 8 \quad 2 \quad 11 \quad 7]^T$$
$$X_2 = [4 \quad 19 \quad 5 \quad 15 \quad 10]^T$$
$$\beta = [2 \quad 3]^T$$

System 2

$$X_1 = [50 \quad 190 \quad 205 \quad 300 \quad 340]^T$$
$$X_2 = [4 \quad 19 \quad 5 \quad 15 \quad 10]^T$$
$$\beta = [0.2 \quad 3]^T$$

$$X = [X_1 \quad X_2]$$

condition number of $X^T X$

75.2	1791.7

variances (model contribution $(X^T X)^{-1}$)

$$\begin{bmatrix} 0.0592 & -0.0333 \\ -0.0333 & 0.0201 \end{bmatrix} \qquad \begin{bmatrix} 1.5837e{-05} & -2.7742e{-04} \\ -2.7742e{-04} & 6.2351e{-03} \end{bmatrix}$$

linear in parameters : well-conditioned

$$\tilde{y} = \begin{bmatrix} 3 & 4 \\ 8 & 19 \\ 2 & 5 \\ 11 & 15 \\ 7 & 10 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \xi$$

$$\xi = N(0,2.0)$$

$$\begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

$$\widehat{\beta_1} = 2 + \delta$$

$$\widehat{\beta_2} = 3 + \delta$$

$$\delta = N(0,0.5)$$

Monte Carlo simulations with 1000 realizations for two set-ups

	Fixed Parameter Without Error Density	Fixed Parameter With Error Density	Analytical solution
Mean of β_2	2.9992±0.1510	2.9998±0.5636	-
Variance of β_2	**0.0057**	**0.0794**	**0.0846**
Mean of β_1	1.9960±0.2623	2.0494±1.6133	-
Variance of β_1	**0.0172**	**0.6507**	**0.7017**

linear in parameters : ill-conditioned

$$\tilde{y} = \begin{bmatrix} 50 & 4 \\ 190 & 19 \\ 205 & 5 \\ 300 & 15 \\ 340 & 10 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \xi$$

$$\xi = N(0{,}2.0) \qquad \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 0.2 \\ 3 \end{bmatrix}$$

$$\widehat{\beta_1} = 0.2 + \delta_1 \qquad \delta_1 = N(0{,}0.05)$$

$$\widehat{\beta_2} = 3 + \delta \qquad \delta = N(0{,}0.5)$$

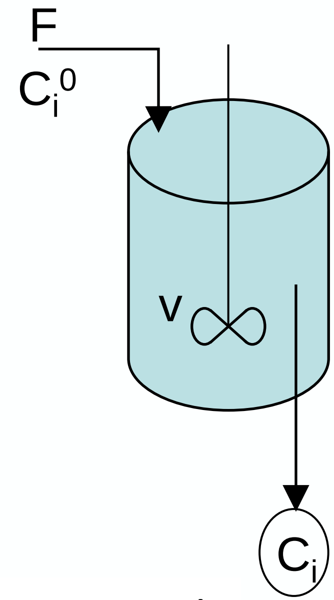
Monte Carlo simulations with 1000 realizations for two set-ups

	Fixed Parameter Without Error Density	Fixed Parameter With Error Density	Analytical solution
Mean of β_2	2.9973±0.1612	3.0096±1.7087	-
Variance of β_2	**0.0065**	**0.7299**	**0.7726**
Mean of β_1	0.2000±0.0001	0.1997±0.0087	-
Variance of β_1	**1.5000E-09**	**1.8900E-05**	**5.0888E-04**

continuous stirred tank reactor

Reaction:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D$$



Data generation:
k_1 = 2.5 sec^{-1}
k_2 = 3.5 sec^{-1}
k_3 = 5.6 sec^{-1}
Measurement error: 3% in output
Volume: 2L
Flow varies from 0.05 – 10 L/sec

C_A^0 =2 mol/L C_B^0 =1 mol/L C_C^0 =0.75 mol/L C_D^0 =0.25 mol/L

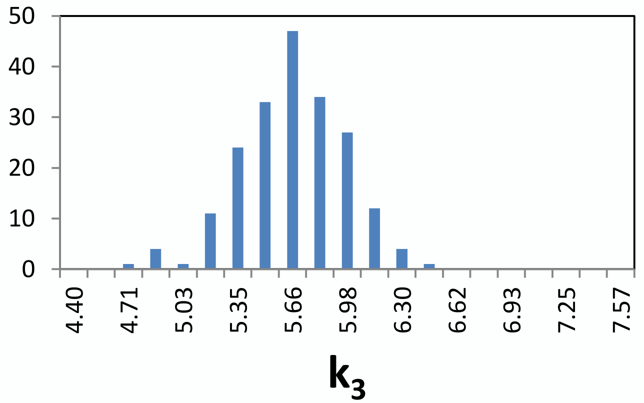
Reactor model:

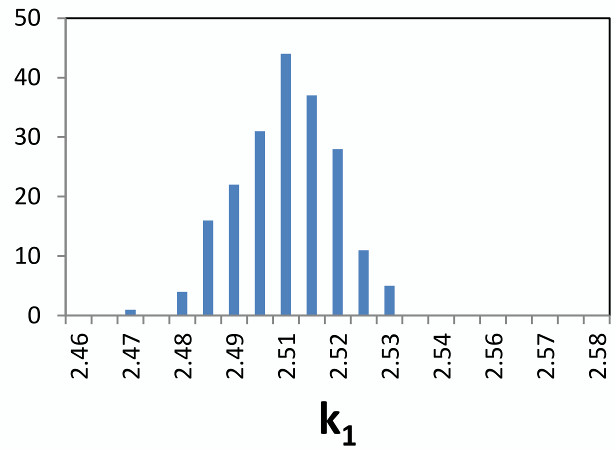
$$F_i^{in} - F_i^{out} + R_i V = 0 \;;\; \text{where } i = A, B, C \text{ and } D$$

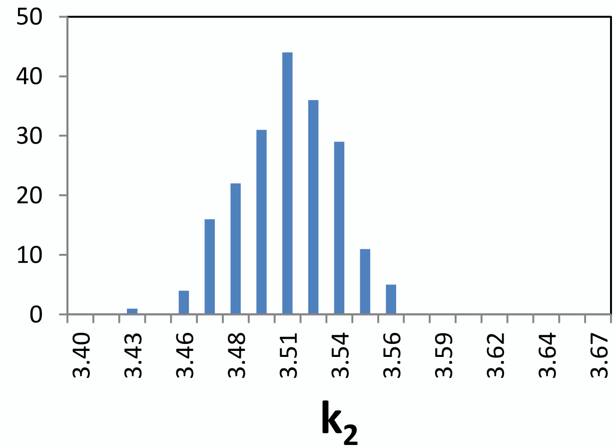
fixed parameter: small variances

$k_3 = 5.6 + \delta \qquad \delta = N(0{,}0.3)$

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D$$



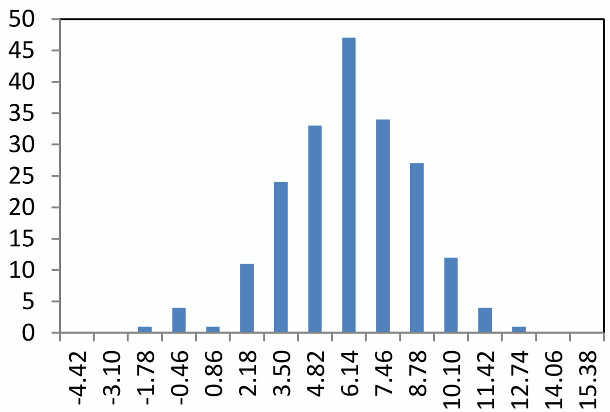




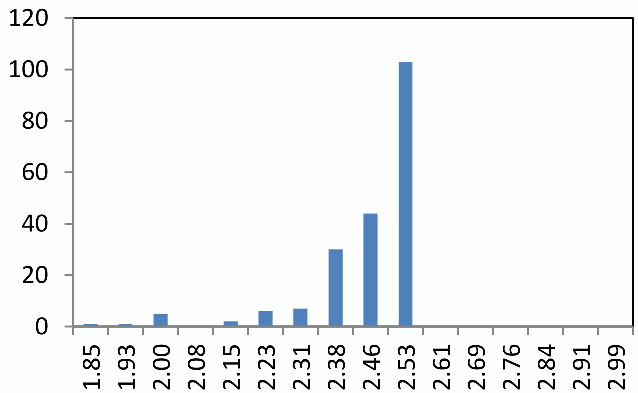
fixed parameter: large variances

$k_3 = 5.6 + \delta \qquad \delta = N(0,2.5)$

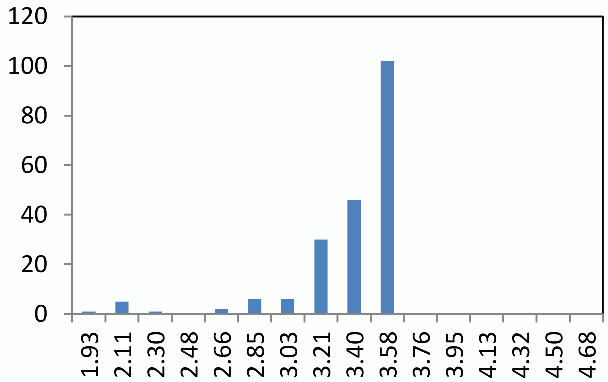
$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D$$



k_3



K_1

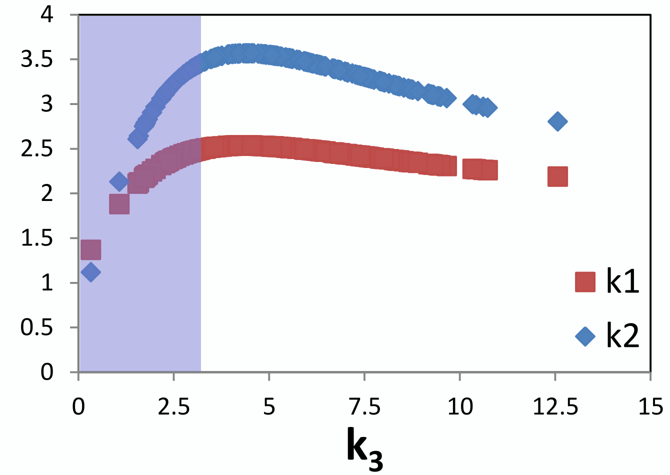


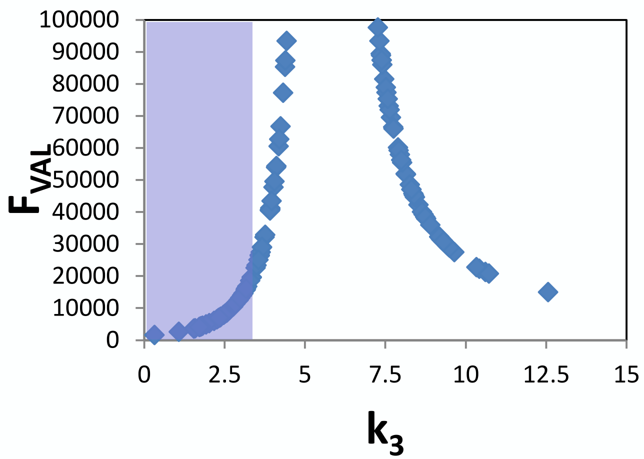
k_2

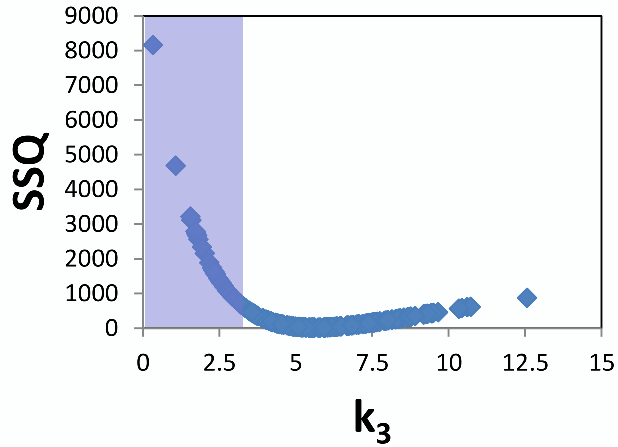
fixed parameter: large variances

$k_3 = 5.6 + \delta \qquad \delta = N(0,2.5)$

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D$$







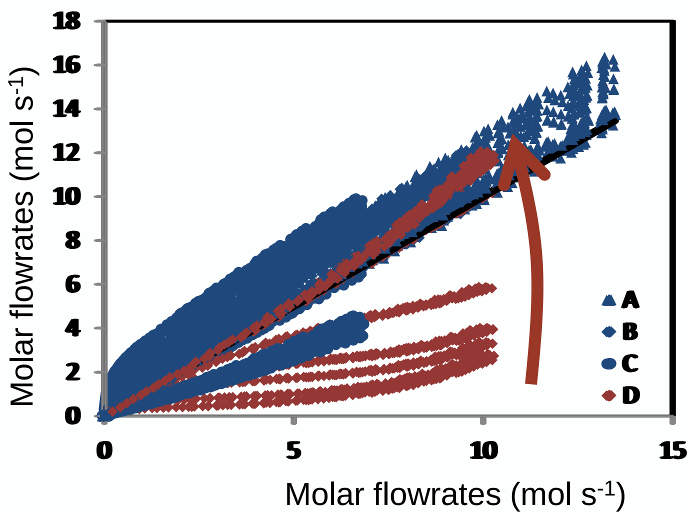
continuous stirred tank reactor

$k_3 = 5.6 + \delta \qquad \delta = N(0,2.5)$

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D$$

k_3 <5.6, third step is rate-determining
- Under predicted products and hence, over predicted reactants

k_3 >5.6, other steps are rate-determining
- No major change in parity



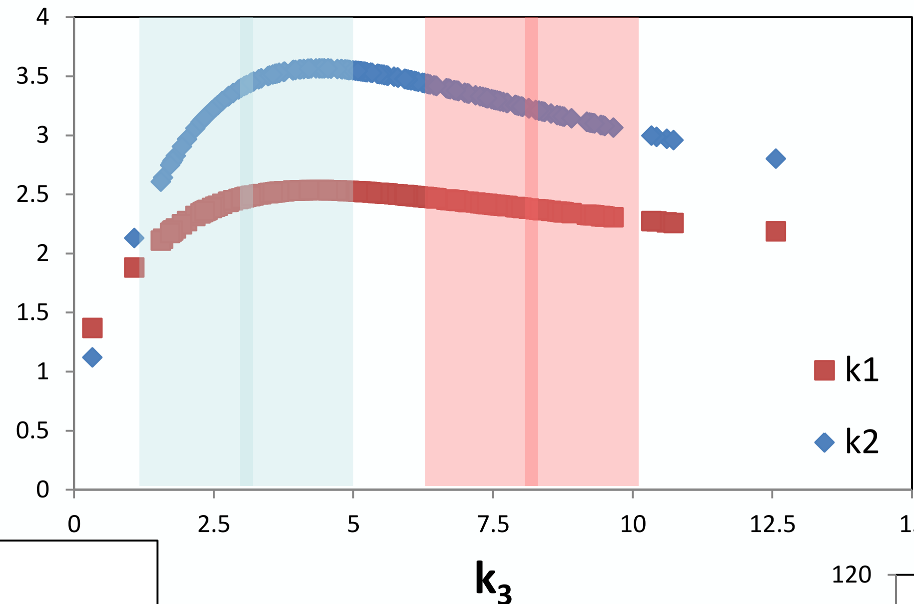
$k_3 = 0.06 \rightarrow 12.96\ sec^{-1}$

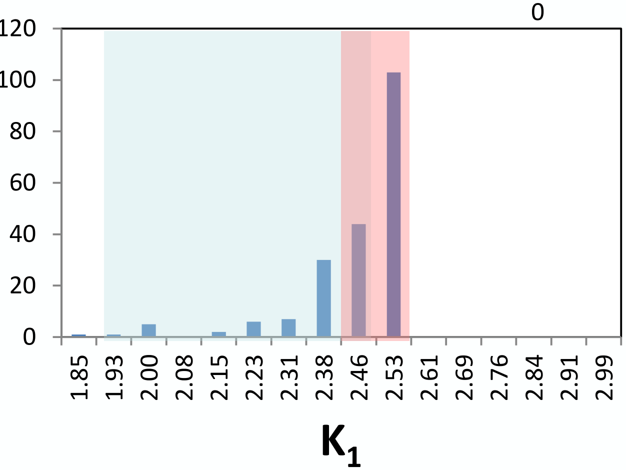
fixed parameter at wrong value

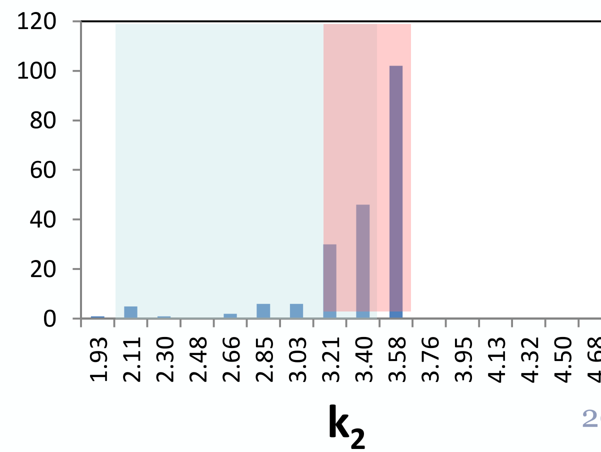
$k_3 = 5.6 + \delta$ $\delta = N(0,2.5)$

$k_3 = 3.0 + \delta$

$k_3 = 8.0 + \delta$







conclusions

- Propagation of errors in the fixed parameters has been studied successfully for linear cases.
- Variances of the estimated parameters are amplified significantly because of the ill conditioning, while for well-conditioned system the propagation is not so pronounced.
- Kinetic example(s) are limited by the reaction behaviour with larger variance in the fixed parameters, while in case of smaller variances, statistics dominates.
- The uncertainties in the fixed parameters should be accounted for in optimal experimental design.

acknowledgements

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Thank you!