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Department of Applied Mathematics, Biometrics and Process Control

A fully automated, iterative procedure to design and (remotely) perform experiments for accurate estimation of nonlinear model parameters

Peter A. Vanrolleghem and Dirk J.W. De Pauw

Cesame Seminar (February 1, 2005)

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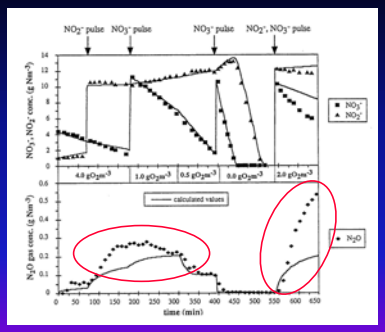
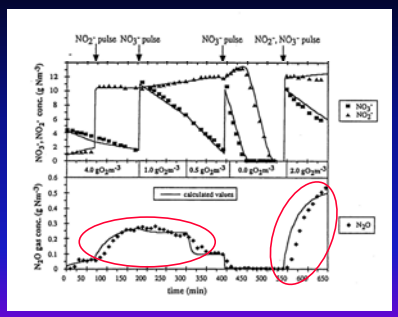
Understanding N_2O emissions



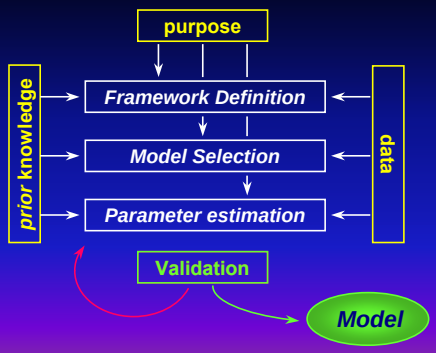
Model is insufficiently "flexible"

Understanding N_2O emissions



Model is much better !

Model building: Subtasks



Outline

- Optimal experimental design (OED)
- Optimization issues and Genetic Algorithms
- An automated procedure
- Practical application to a hybrid respirometer
- A posteriori analysis of results
- Conclusions

Optimal experimental design

- What ?

  A mathematical technique to design an experiment in such a way that it produces data with a maximal information content

- Why ?
  - More accurate parameter estimation
  - Limited resources (time and money)
  - Large # of experimental degrees of freedom

Optimal experimental design

- How ?

Fisher Information Matrix (FIM)
(measure for the information content of the experiment)

$$FIM = \sum_{i=1}^{N} \left(\frac{\partial y}{\partial \theta}\right)_i^T Q_i^{-1} \left(\frac{\partial y}{\partial \theta}\right)_i$$

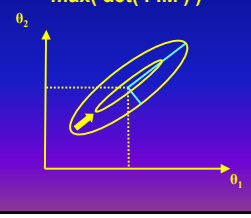
(local) sensitivity functions

measurement error covariance matrix

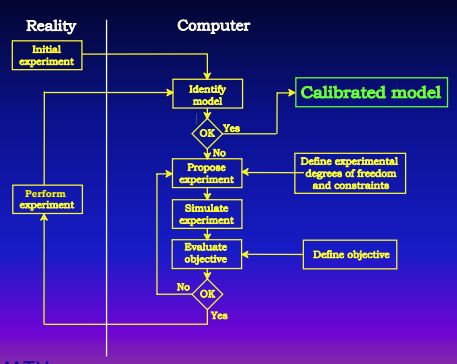
Define objective

Minimizing / maximizing properties of the FIM
➡ **relates to parameter estimation confidence information**

D criterion (volume):
max(det(FIM))



Classical iterative design procedure



(adapted from Dochain and Vanrolleghem, 2001)

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The use of genetic algorithms in parameter estimation and optimal experimental design problems

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Outline

- Classical genetic algorithms
- Real-value genetic algorithms
- Use of GA's in calibration
- Use of GA's in experimental design
- Conclusions

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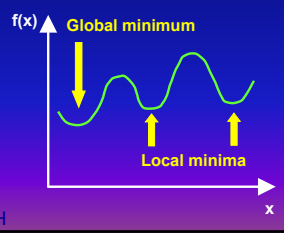
Classical genetic algorithms

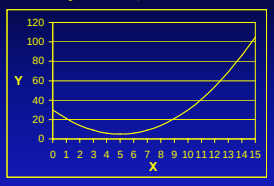
- What ?

Global optimization algorithms inspired on the genetic processes of natural evolution



Problem formulation

- Example: $y = x^2 - 10x + 30$



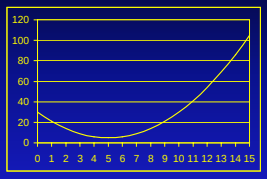
Find integer x which minimizes y

- Encoding:

Problem 0-15 ➡ GA (binary) 0000-1111

Initial population

	x	y
1101	13	69
0001	1	21
0111	7	9
1100	12	54
1111	15	105



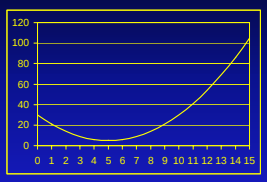
1

Selection, crossover and mutation

	x	y				x	y
1101	13	69					
0001	1	21	➡	0001	➡ 0011	3	9
0111	7	9	➡	0111	➡ 0101	5	5
1100	12	54					
1111	15	105	➡	1111	➡ 0111	7	9

Next generation

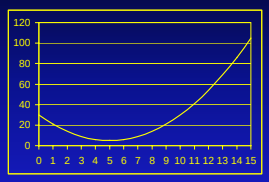
	x	y
0011	3	9
0101	5	5
0111	7	9
1010	10	30
0011	4	6



1
2

Final generation

	x	y
0101	5	5
0101	5	5
0101	5	5
0101	5	5
0101	5	5



1
2
:
N

Binary encoding problems

- Difficulties associated with binary encoding:
  - continuous search spaces
  - large dimension
  - great numerical precision
- Example:
  - [-500, 500]
  - 100 variables
  - 6 digits after the decimal point

➡ chromosome of size 3000

➡ search space $\pm 10^{1000}$

Outline

- Classical genetic algorithms
- Real-value genetic algorithms
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Real-value genetic algorithms

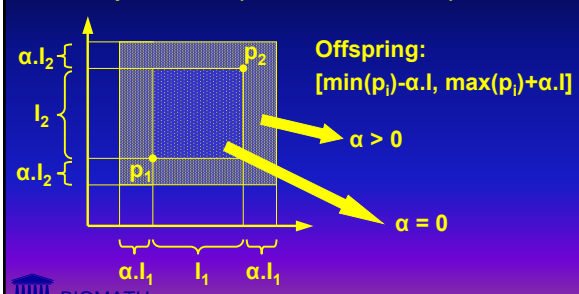
- Directly encode variables as real-values

➡ Each gene represents one variable

- Advantages:
  - large domains
  - high precision / local tuning
  - close to the problem formulation
- Disadvantage:
  - redefine crossover and mutation operators

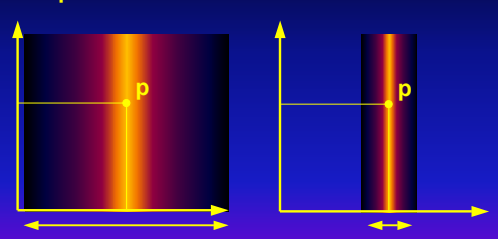
Real-value crossover

- Many operators exist (± 10-20)
- Example: BLX-α (blended crossover)



Real-value mutation

- Also many operators exist (± 10)
- Example: Non-uniform mutation



also adaptive: based on generation number

Practical considerations

- GA tuning:
  - genetic algorithm type
  - genetic algorithm encoding
  - population size
  - choice of crossover / mutation operator
  - crossover / mutation probabilities
  - crossover / mutation tuning parameters
- GA control:
  - change GA settings during execution

➡ More art than science !!!

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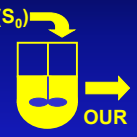
Optimization example

- OUR example:

Batch reactor: S + O --> X

Substrate (S_0)



$$\frac{dS}{dt} = -\frac{1}{Y}\frac{\mu S}{K_S + S}X$$

$$OUR = \frac{1-Y}{Y}\frac{\mu S}{K_S + S}X$$

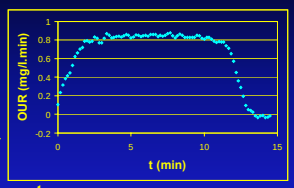
➡ Estimate Monod kinetics parameters μ_{max} and K_S

Optimization example

- OUR example:

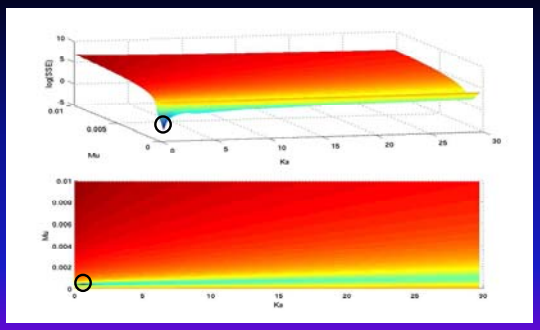
Batch reactor:

Substrate (S_0)



➡ Estimate Monod kinetics parameters μ_{max} and K_S

OUR objective surface



Optimum: μ_{max}: 0.00042 min^{-1}

K_S: 0.44 $mg.l^{-1}$

GA performance

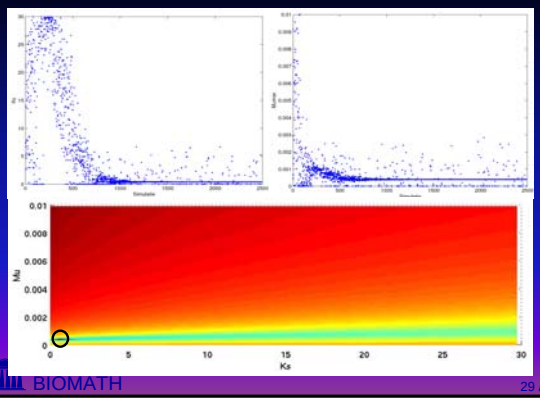


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Illustration

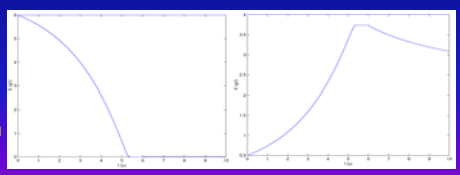
- Fed-batch reactor

Substrate (S_0)
$t = 0$

$t > t_f$: Pump speed Q_f
Feed concentration S_f

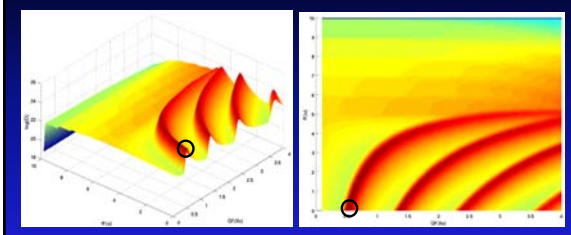
Measure S and X
(interval = 1 h)

$S_0 = 6\ g.l^{-1}$
$t_f = 6\ h$
$Q_f = 4\ l.h^{-1}$
$S_f = 10\ g.l^{-1}$



D-criterion: 1.29E+22

D-criterion objective surface



Optimum: $t_f = 0\ h$
$Q_f = 0.53\ l.h^{-1}$

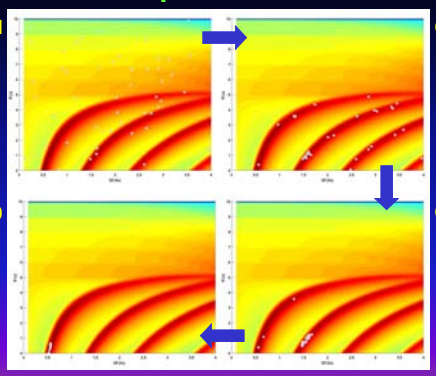
GA performance

Gen.1

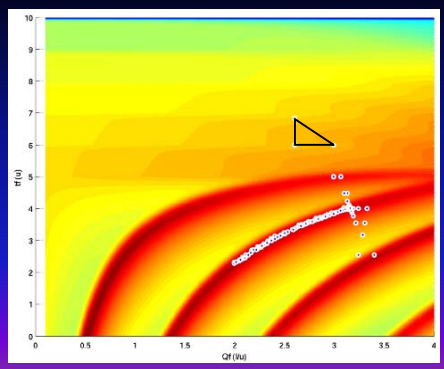
Gen. 9

Gen. 39

Gen. 17



Simplex performance



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Conclusions

- Binary vs. real encoding:
  Real encoding outperforms binary encoding for complex problems
- GA's in general:
  + global search !!!
  + can also be used with discrete variables
  - difficult to tune: case specific
  - large number of objective evaluations
  - slow convergence ➡ hybrid optimization algorithms

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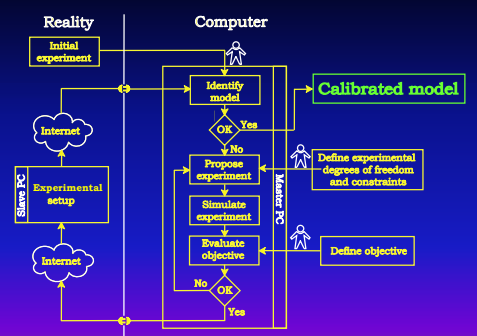
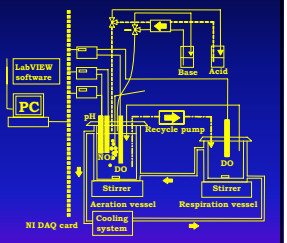
An automated iterative procedure



BIOMATH (adapted from Dochain and Vanrolleghem, 2001) 38 / 25

Experimental setup

Hybrid respirometer (Sin *et al*. 2003)



DO measurements → Oxygen uptake rate (OUR)

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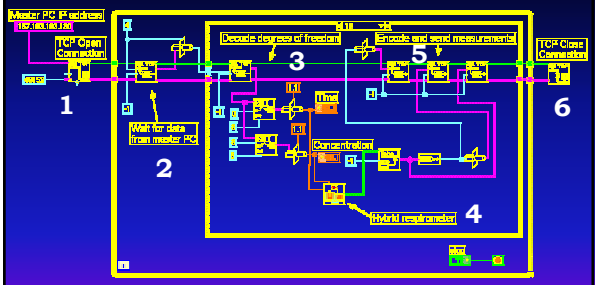
Communicating with LabVIEW



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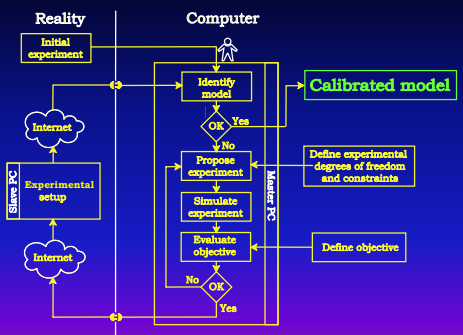
An automated iterative procedure



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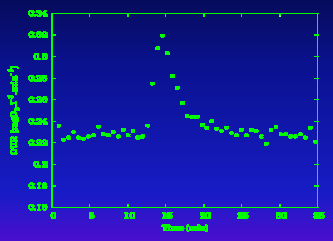
Identify model from initial experiment

- **Initial experiment:**

pulse of 0.5 mg NH_4^+ added to the aeration vessel at 12 minutes after the start of the experiment



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Identify model from initial experiment

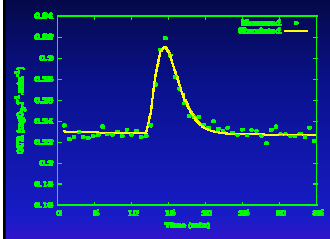
- Model: one-step nitrification

exogenous OUR

$$OUR = \frac{4.57 - Y_{NH4}}{Y_{NH4}} \times \left(1 - e^{-\frac{t - t_{pulse}}{\tau}}\right) \times \mu_{max,NH4} \times \frac{S_{NH4}}{K_{NH4} + S_{NH4}} \times X_{NH4}$$

Identify model from initial experiment

- Model calibration:

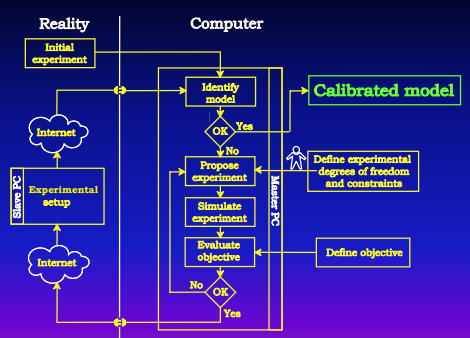


Parameter estimation errors:

Name	Estimation errors (% of parameter value)
$\mu_{max,NH4}$	927
K_{NH4}	5118
Y_{NH4}	4682
τ	106

➡ Optimal experimental design is needed

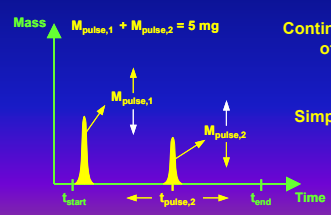
An automated iterative procedure



(adapted from Dochain and Vanrolleghem, 2001)

Define experimental degrees of freedom and constraints

- Two pulse additions of NH_4^+ added by a pump to the aeration vessel
- First pulse always added at start of experiment
- Total added mass = 5 mg NH_4^+ (Grady *et al.*, 1996)
- Total experimental time = 110 minutes

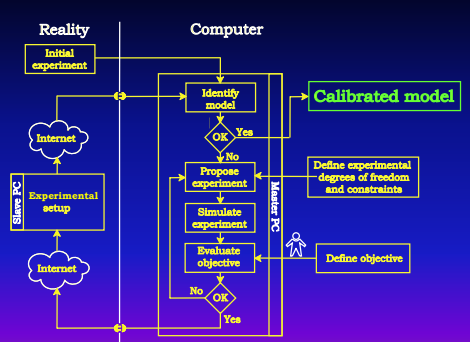


Continuous degrees of freedom

➡

Simplex optimizer

An automated iterative procedure



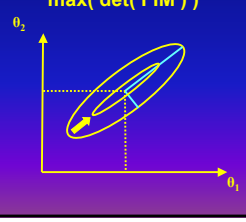
(adapted from Dochain and Vanrolleghem, 2001)

Define objective

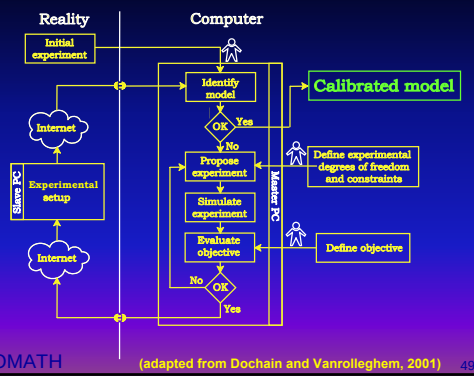
Minimizing / maximizing properties of the FIM

➡ relates to parameter estimation confidence information

D criterion (volume):
max(det(FIM))



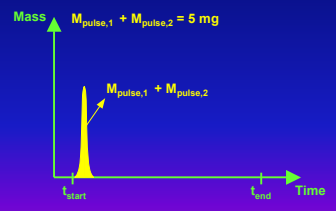
An automated iterative procedure



(adapted from Dochain and Vanrolleghem, 2001)

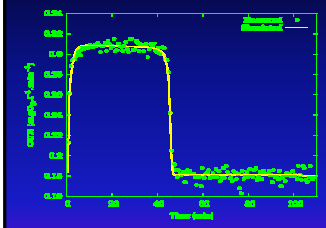
First designed experiment

- **Optimal experiment:**
  - All 5 mg NH_4^+ in first pulse
  - D-criterion value = 2.07E+15



First designed experiment

- **Calibration results:**

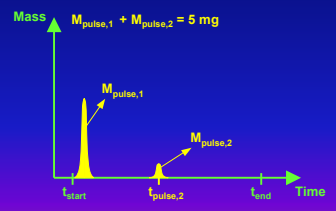


Parameter estimation errors:

Name	Estimation errors (% of parameter value)
$\mu_{max,NH4}$	3.44 [927]
K_{NH4}	21.1 [5118]
Y_{NH4}	3.40 [4682]
τ	10.9 [106]

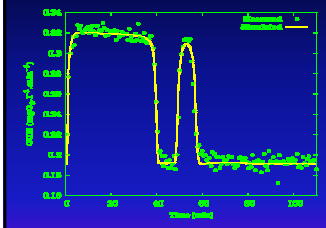
Second designed experiment

- **Optimal experiment:**
  - 4.17 mg NH_4^+ at start and 0.83 mg at 48.32 minutes
  - D-criterion value = 1.26E+23 [2.07E+15]



Second designed experiment

- **Calibration results:**

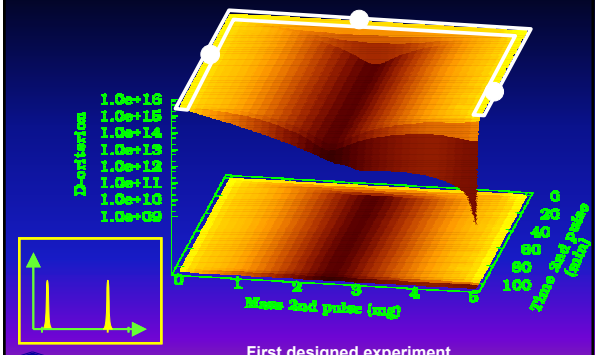


Parameter estimation errors:

Name	Estimation errors (% of parameter value)
$\mu_{max,NH4}$	6.47 [3.44]
K_{NH4}	23.3 [21.1]
Y_{NH4}	6.50 [3.40]
τ	11.6 [10.9]

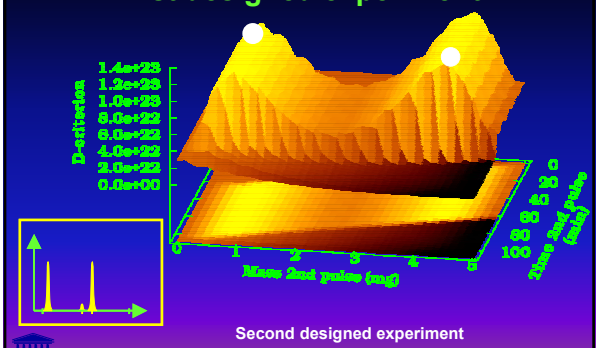
➡ End of experimental design procedure

Objective surface for initial experiment



First designed experiment

Objective surface for first designed experiment



Second designed experiment

Conclusions

- An automated iterative procedure for optimal experimental design was developed and successfully applied.
- The procedure can easily be applied to any experimental setup controlled by a LabVIEW VI.
- The iterative nature of the procedure has shown to be very robust to the nominal parameter values.

Any questions ?