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Optimal experiment design using sequential semidefinite programming

D. Telen, F. Logist, R. Quirynen, B. Houska, M. Diehl and J. Van Impe

Overview

Introduction

Optimal experiment design

Semidefinite programming

Proposed algorithm

Simulation results

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General introduction

Mathematical model of a process?

“an approximate representation of a real-world process”



$$\frac{dy(t)}{dt} = g(y(t), p, u(t))$$

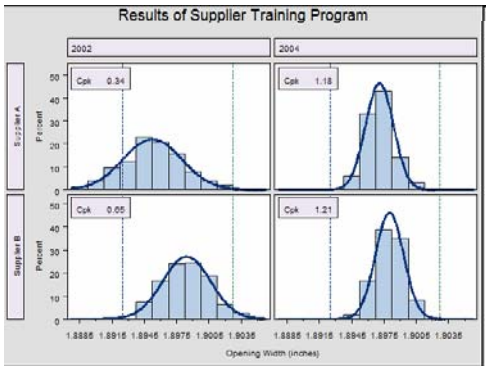
General introduction

Why model a process?

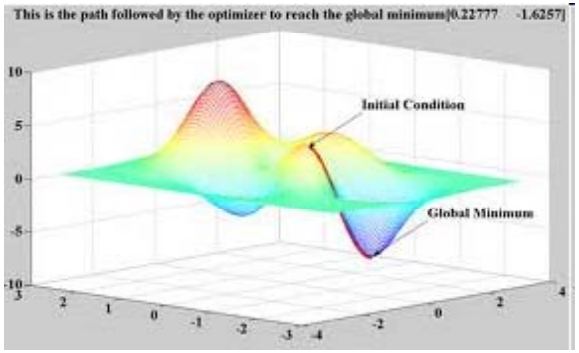
- Analyze process behavior

- Control the process

- Optimize process operation







General introduction

What kind of model?

White-box models

- based on the underlying physical, chemical, ... mechanisms
- require deep process insight

also called ***first-principle*** or ***mechanistic*** models

Constructing the model

Data required ... but experiments are

- costly
- labor intensive
- potentially hazardous

Need for ***Optimal experiment design***

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Quantifying the information content

The Fisher information matrix:

$$F(t_f) = \int_0^{t_f} \frac{\partial y(t)}{\partial p}^T C(t)^T Q(t)^{-1} C(t) \frac{\partial y(t)}{\partial p} dt$$

consists of:

$\frac{\partial y(t)}{\partial p}$: sensitivity of the model wrt the parameters

$C(t)$: derivative of the $h(y(t))$ wrt $y(t)$

$Q(t)^{-1}$: inverse variance-covariance measurement errors

Optimal experiment design

Optimizing the information content

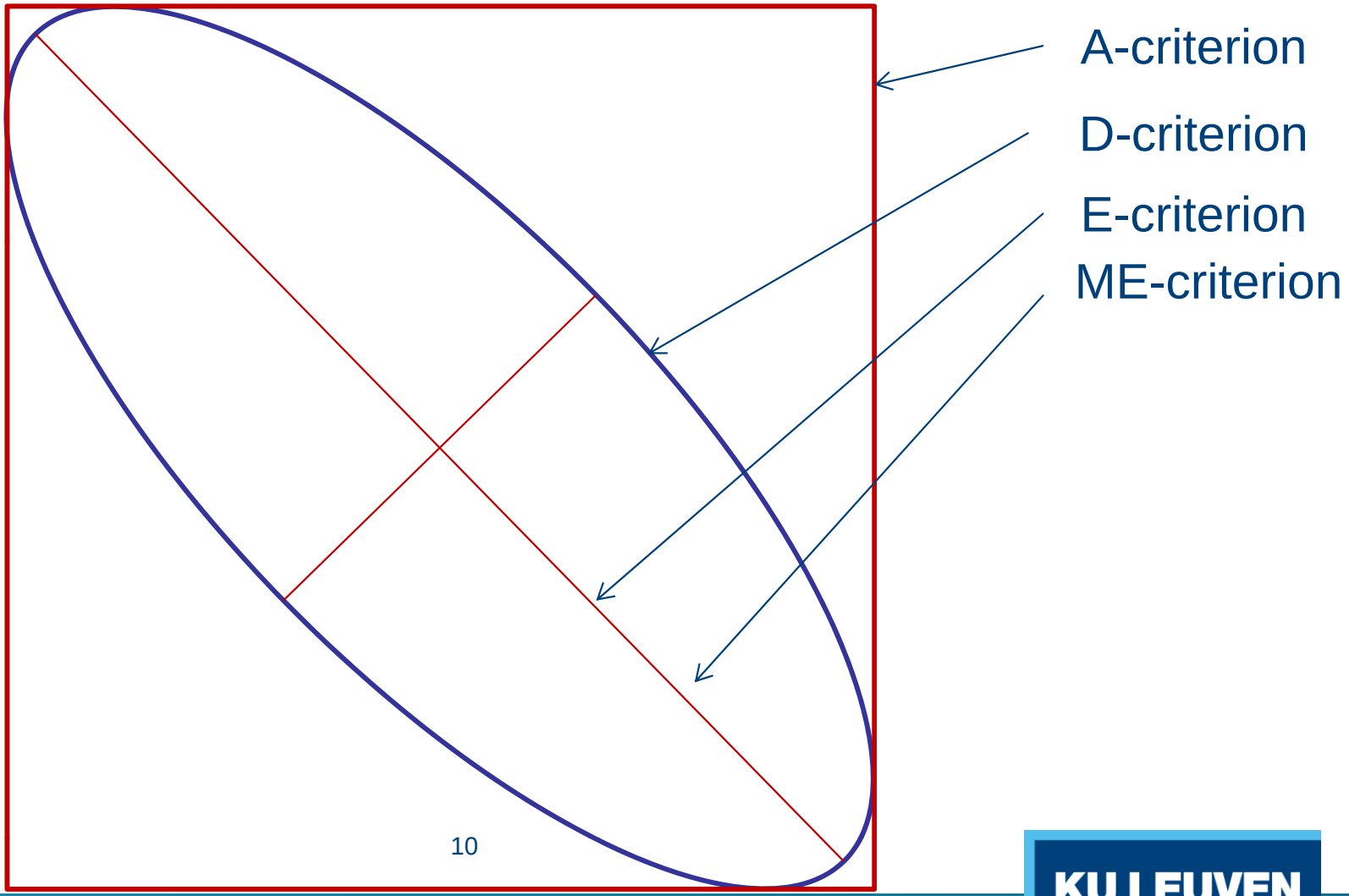
Optimizing a matrix is not possible → need of a scalar map

Different scalar functions:

- A-criterion: min (trace $F(t_f)^{-1}$)
- D-criterion: max (det $F(t_f)$)
- E-criterion: max ($\lambda_{min}(F(t_f))$)
- Modified E-criterion: min ($\lambda_{max}(F(t_f))/\lambda_{min}(F(t_f))$)

Optimal experiment design

The different scalar functions



Optimal experiment design

Issues with specific objective functions

Derivative does not always exist

→ needed for Newton type optimization schemes

Presence of matrix inverse

→ challenge for the accurate computation of derivatives

Several criteria to choose

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Mathematical problem formulation

$$\min c^T \xi$$

subject to:

$$K(\xi) \succcurlyeq 0$$

$$\text{with } K(\xi) = K_0 + \sum_{i=1}^{m} K_i \xi_i$$

here K_i denotes symmetric matrices

and $K(\xi) \succcurlyeq 0$ means positive semidefinite, i.e.,

$\forall z: \; z^T K(\xi) z \geq 0$

Problem is convex optimization problem

Can be solved efficiently: both in theory and practice

Semidefinite programming

Interesting case of semidefinite programming

$$\min \quad -\tau$$

subject to:

$$K(\xi) - \tau I \succcurlyeq 0$$

$$\text{with } K(\xi) = K_0 + \sum_{i=1}^{m} K_i \xi_i$$

here K_i denotes symmetric matrices

and $K(\xi) \succcurlyeq 0$ means positive semidefinite, i.e.,

$\forall z: \; z^T K(\xi) z \geq 0$

→ Maximization smallest eigenvalue of $K(\xi)$

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Linearize the Fisher information matrix

For a given u_k, approximate the Fisher information matrix as:

$$F_k(t_f, u, u_k) = F_k(t_f, u_k) + \frac{\partial F_k(t_f, u_k)}{\partial u}(u - u_k)$$

Semidefinite problem solved in each iteration

Maximization of the smallest eigenvalue

$$\min \quad -\tau$$

subject to:

$$F_k(t_f, u, u_k) - \tau I \succcurlyeq 0$$

Proposed algorithm

Avoid the explicit formulation of matrix inverse (A-criterion)

Cast in the SDP framework

$$\min \quad trace(X)$$

subject to:

$$X \succcurlyeq F_k(t_f, u, u_k)^{-1}$$

where X is an additional matrix decision variable

Reformulated

$$\min \quad trace(X)$$

subject to:

$$\begin{bmatrix} F_k(t_f, u, u_k) & I \\ I & X \end{bmatrix} X \succcurlyeq 0$$

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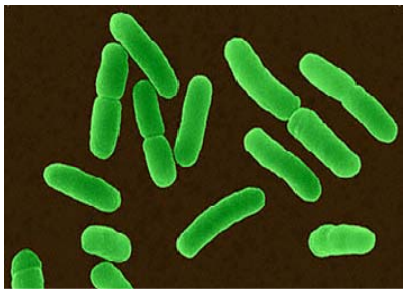
Predictive microbial growth model (*E. coli*)

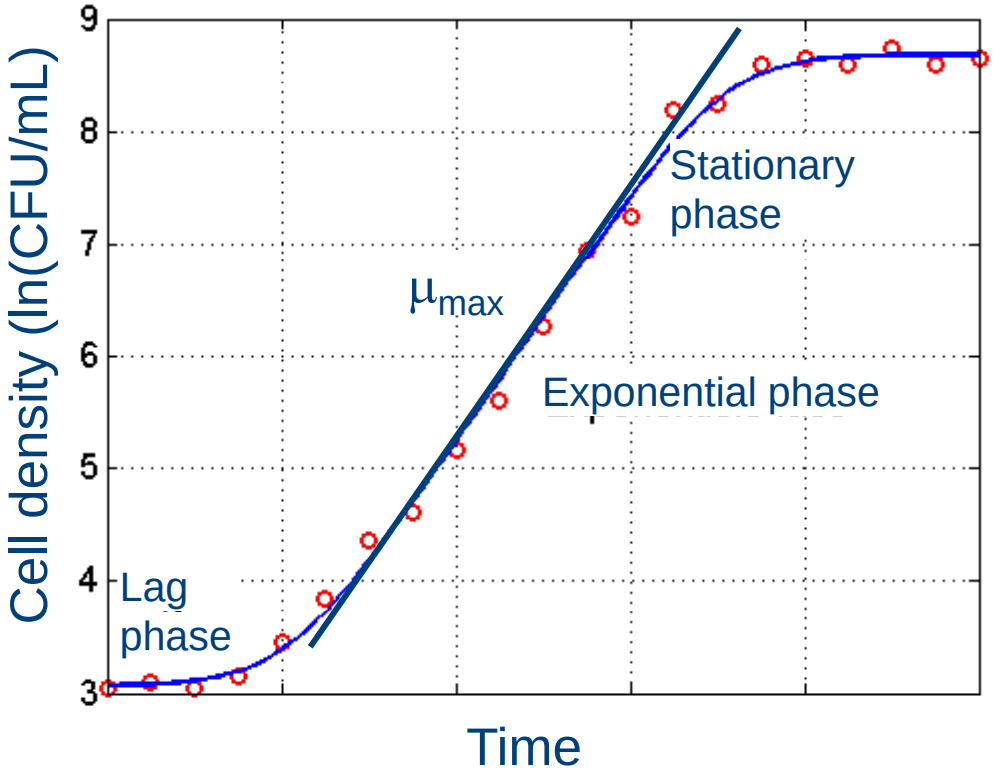
Model equations

$$\frac{dn(t)}{dt} = \frac{Q(t)}{Q(t)+1}\mu_{max}(T(t))\left[1 - exp^{n(t)-n_{max}}\right]$$

$$\frac{dQ(t)}{dt} = \mu_{max}(T(t))Q(t)$$





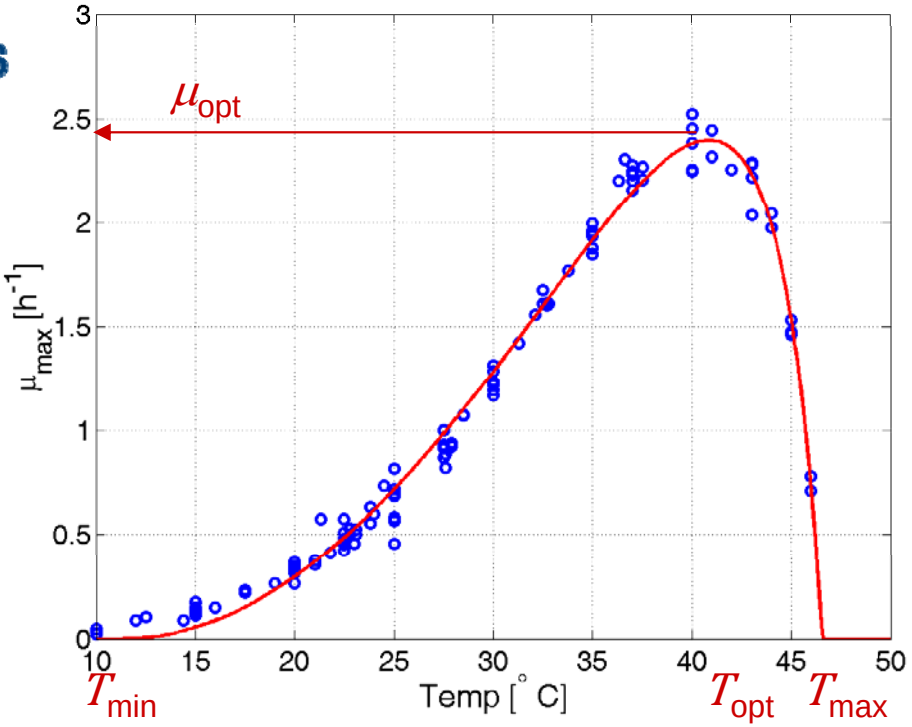


Simulation results

Secondary model describing temperature dependency

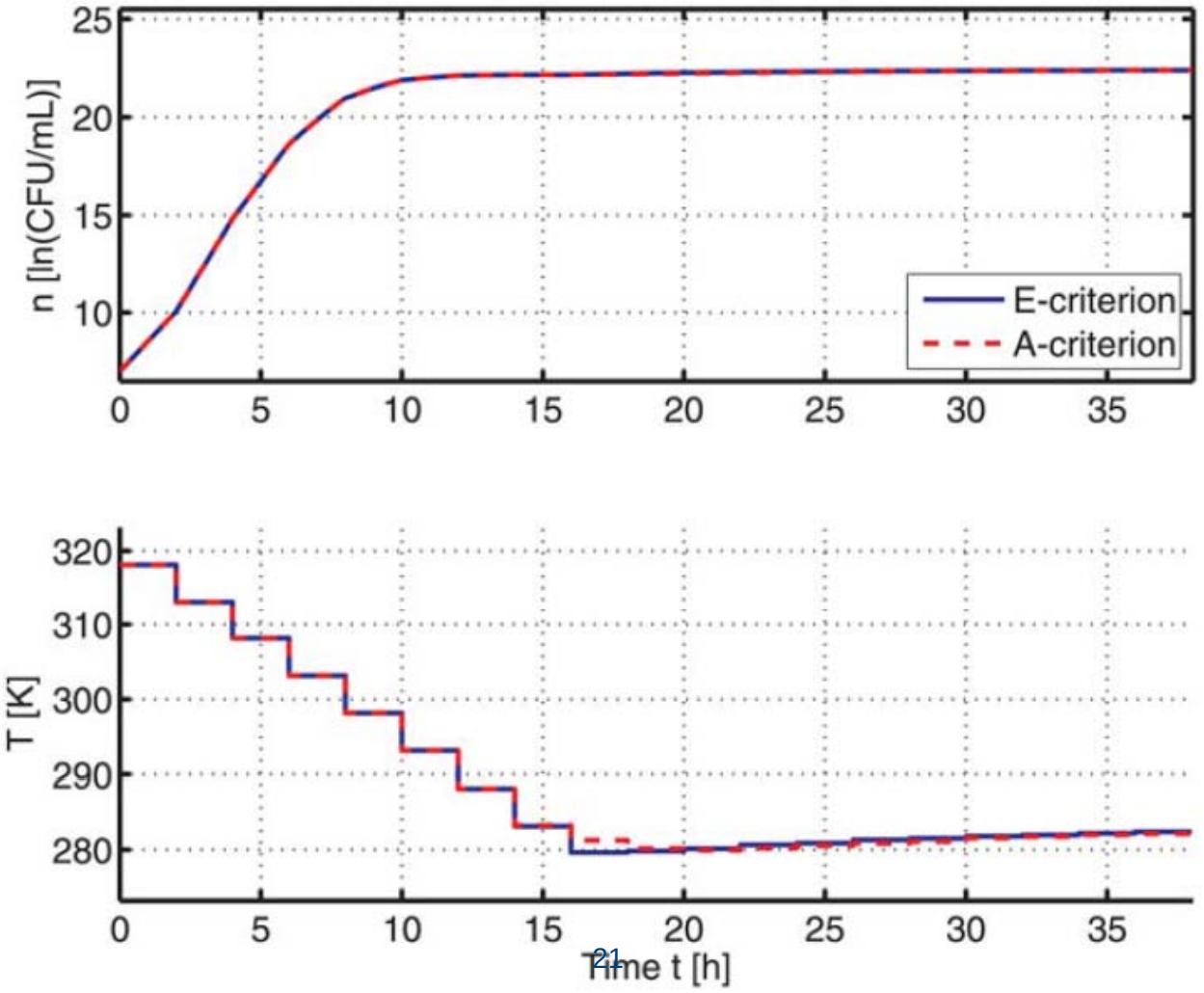
$$\mu_{max}(T(t)) = \mu_{opt} \frac{(T(t) - T_{min})^2 (T(t) - T_{max})}{(T_{opt} - T_{min})[(T_{opt} - T_{min})(T(t) - T_{min}) - (T_{opt} - T_{max})(T_{opt} + T_{min} - 2T(t))]}$$

Four parameters



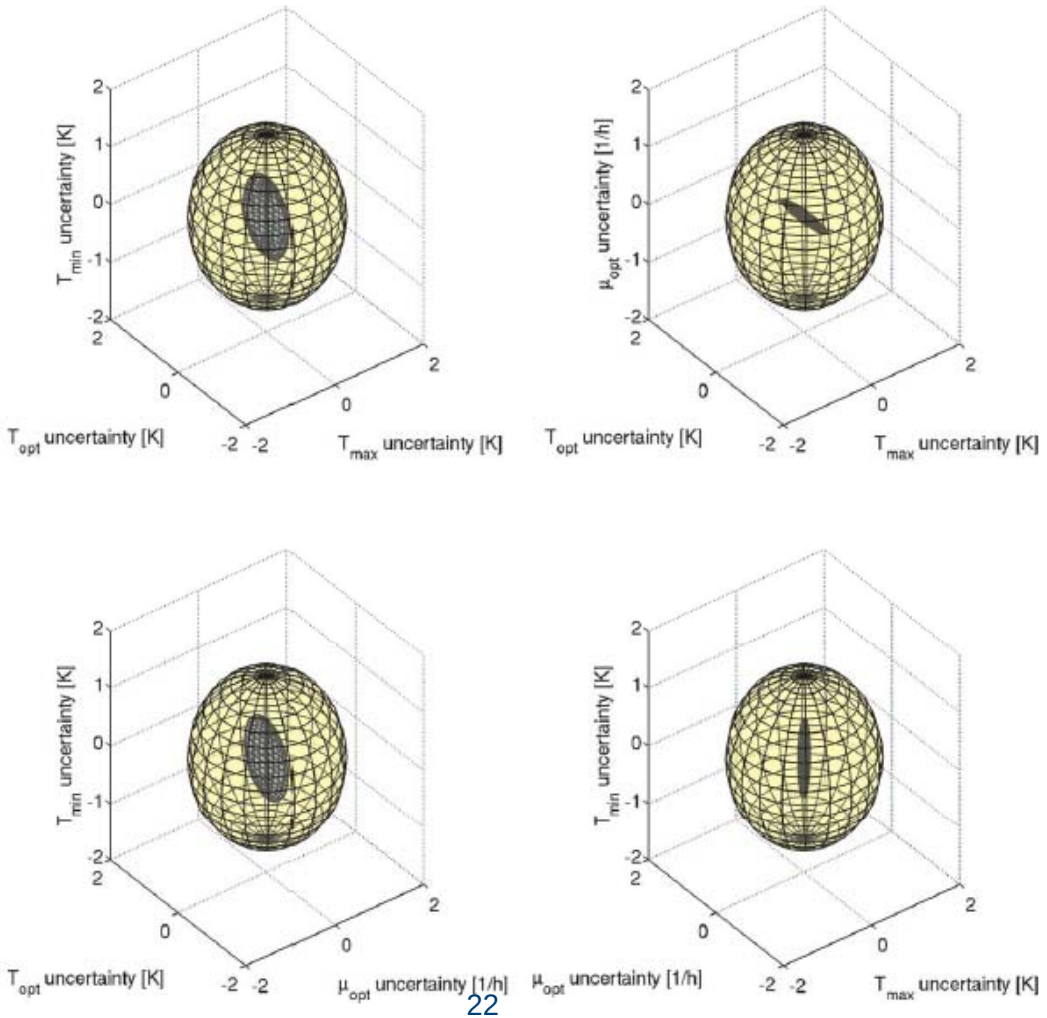
Simulation results

A- and E-optimal experiments



Simulation results

Predicted 3D joint confidence regions



Conclusions

Novel algorithm for OED by sequential SDP

Easy formulation of minimal eigenvalue maximization

Problems with inverse of Fisher information matrix are avoided

Presented methodology illustrated to biochemical case study

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