A closed loop identification software for dynamic systems: ODOE4OPE (Optimal Design Of Experiments for Online Parameter Estimation)

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\(^3\)Project leader and contact. Software website: http://odoe4ope.univ-lyon1.fr

Journée nationale des logiciels de modélisation et de calcul scientifique (LMCS):
07/12/2012
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- Synthesizes the online design of the optimal experiment (DOE) and online closed-loop identification.
- For linear and nonlinear dynamic model based systems.
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- Online optimal input design which optimizes the sensitivities of the measurements with respect to the unknown constant model parameters.

Proposed closed-loop optimal identification approach

Stage of development

Case study: Bio-reactor

Conclusion

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Closed loop control structure

- Process
- Observer
- Model
- Sensitivity Model

The components:
- 

http://odoe4ope.univ-lyon1.fr
The components

Model (linear or nonlinear)

\[
(M) \begin{cases}
\dot{x}(t) &= f(x(t), \theta, u(t)) \\
y(t) &= h(x(t), \theta, u(t))
\end{cases}
\]  

(1)

where \( x \in \mathbb{R}^n \) is the state vector, \( y \in \mathbb{R}^p \) is the output vector, \( u \in \mathcal{U} \subset \mathbb{R}^m \) is the input vector, \( \theta \in \mathbb{R}^q \) is the unknown constant parameters vector.

Observer

- system augmented with the unknown constant model parameters.
- synthesis of an observer for the system augmented: high gain observer, EKF, adaptive-gain observer, ...
The components

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Sensitivity model

\[
(M_\theta) \begin{cases}
\frac{\partial \tilde{x}_\theta}{\partial t} &= \frac{d}{dt} \left( \frac{\partial x}{\partial \theta} \right) = \frac{\partial}{\partial \theta} \left( \frac{\partial x}{\partial t} \right) = \frac{\partial f}{\partial \theta} + \frac{\partial f}{\partial x} \frac{\partial x}{\partial \theta} \\
\frac{\partial \tilde{y}_\theta}{\partial \theta} &= \frac{\partial h}{\partial \theta} + \frac{\partial h}{\partial x} \frac{\partial x}{\partial \theta} + \frac{\partial y}{\partial x} \frac{\partial x}{\partial \theta}
\end{cases}
\]
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\frac{\partial y}{\partial \theta} = \tilde{y}_\theta = \frac{\partial h}{\partial \theta} + \frac{\partial h}{\partial x} \frac{\partial x}{\partial \theta}
\end{array} \right. 
\]

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Optimal control law design

- **Sensitivity matrix:**

  \[ Z_k = \begin{bmatrix}
  \frac{\partial x_1}{\partial \theta_1} |_k & \frac{\partial x_1}{\partial \theta_2} |_k & \cdots & \frac{\partial x_1}{\partial \theta_p} |_k \\
  \frac{\partial x_2}{\partial \theta_1} |_k & \ddots & \ddots & \vdots \\
  \vdots & \ddots & \ddots & \vdots \\
  \frac{\partial x_n}{\partial \theta_1} |_k & \cdots & \cdots & \frac{\partial x_n}{\partial \theta_p} |_k
  \end{bmatrix} \]  

- **Fisher Information Matrix (FIM):**  
  \[ M_k = Z_k^T Z_k \]

- **Cost function**

  \[
  J = \phi(F(x_j|k, u_j|k, \theta_k|k)),
  \]

  with

  \[
  F(x_j|k, u_j|k, \theta_k|k) = \frac{1}{N_p} \sum_{j=k+1}^{k+N_p} M_j|k
  \]

- **Criterion: A-optimality**

  \[
  \left\{ \begin{array}{l}
  u = \arg \max_{u \in [u_{min}, u_{max}]} J_A(u) \\
  \text{with } J_A(u) = \text{trace}(F)
  \end{array} \right. \]
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History: created in 2009

Fundamentals Aspects:
- 2006-2010: Saida Flila’s PhD thesis
- Mars 2012: PhD thesis CIFRE (J. QIAN) between Acsystème and LAGEP (UMR5007, CNRS, UCBL1)

User interface: under Matlab, GUI under development
The nonlinear model of Bio-reactor: $X + S \rightarrow X$

The nonlinear dynamical model of the process is:

$$\begin{align*}
\dot{X}(t) &= \frac{\mu_{\text{max}} S(t)}{S(t) + K} X(t) - D(t) X(t) \\
\dot{S}(t) &= -\alpha \frac{\mu_{\text{max}} S(t)}{S(t) + K} X(t) - D(t) (S(t) - S_{in}) \\
y(t) &= X(t).
\end{align*}$$

(Σ)

where:

- Inputs: a scalar controllable dilution rate $D(t) (h^{-1})$ and an substrate concentration $S_{in} (g/L)$.
- Output: a biomass $X(t) (g/L)$
- Unknowns constants parameters: $\mu_{\text{max}}$ and $\alpha$.
- input constraints: $0 h^{-1} \leq D(j) \leq 0.2 h^{-1}$
- output constraint: $X(j) \leq 1.95 g/L$

Objective: based on (Σ) online identify the unknowns parameters.
Simulation results

- Input applied: $D(t)$
Simulation results

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- Process output: Biomass $X(t)$
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Simulation results

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Simulation results

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- Process output: Biomass $X(t)$
- Parameter estimation: $\mu_{\text{max}}$
- Parameter estimation: $\alpha$

![Simulation results graph](http://odo4ope.univ-lyon1.fr)
Simulation results

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![Graph showing simulation results](http://odoe4ope.univ-lyon1.fr)
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![Graphs showing sensitivity states](attachment://graphs.png)
Conclusion

- ODOE4OPE is able to design online the optimal experiment under constraints.
- ODOE4OPE is able to identify online model parameters.
- The combination of an observer and a predictive control in closed loop improve the speed of the parameter estimation.
- The sensitivity criteria improve the accuracy of parameter estimation and leads to an optimal control at the same time.
- The input and output constraints specify the physical limitations imposed by the system and ensure the efficiency of the DOE.
- The software may be adapted and tuned for any user defined dynamic model.
A Model Predictive Control software: MPC@CB

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Main features of the MPC@CB software

- A control software for dynamic systems based on any kind of model: SISO or MIMO (S=single, M=multiple), linear or nonlinear, time variant or time invariant, with ordinary differential equations (ODE) and/or partial differential equations (PDE).

- A model predictive control (MPC) strategy for solving an optimal control problem (trajectory tracking, processing time minimization, any user defined criteria ...) with input constraints and with (or without) output constraints.

http://MPCatCB.univ-lyon1.fr/
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MPC: general framework

- MPC scheme

- Past

- Future

- Reference Trajectory

- Prediction Horizon

- Sample Time

- k

- k+1

- k+2

- ...
MPC: general framework

- MPC scheme

![MPC Scheme Diagram]

- Reference Trajectory
- Past Control Input
- Prediction Horizon
- Sample Time
- Past
- Future

MPC scheme

PAST

FUTURE

k
k+1
k+2
...
k+Np
MPC: general framework

- **MPC scheme**

![Diagram of MPC scheme](image)

- Reference Trajectory
- Measured Output
- Past Control Input

**Sample Time**
MPC: general framework

- MPC scheme

![MPC Scheme Diagram](image-url)
MPC: general framework

- MPC scheme

![MPC Scheme Diagram](https://MPCatCB.univ-lyon1.fr/)

- Reference Trajectory
- Predicted Output
- Measured Output
- Predicted Control Input
- Past Control Input

Sample Time

k  k+1  k+2  ...  k+Np
MPC: general framework

- MPC scheme

![MPC scheme diagram](image_url)
MPC@CB is based on an internal model control (IMC) structure where:

- Nonlinear model $S_0$ is solved off-line.
- Time-varying linearized model $S_{TVL}$ (obtained from $S_0$) is solved on-line.
- Off-line open loop results are used on-line for the correct closed loop optimal constrained tuning of the control action.
Formulation of the optimization problem solved in a MPC approach

\[
\min_p J_{tot} = J(p) + J_{ext}(p) \\
J(p) = \sum_{j=k+1}^{k+N_p} g(y_{ref}(j), \Delta y_m(j), \Delta u(p(j)), e(k)) \\
J_{ext}(p) = \sum_{j=k+1}^{k+N_p} (\sum_{i=1}^{N_c} w_i \max^2(0, c_i(y_{ref}(j), \Delta y_m(j), \Delta u(p(j)), e(k)))) \\
p: \text{unconstrained input parameter} \\
c_i: \text{output constraints for the controlled variables} \\
\text{Input constraints handling: hyperbolic transformation} \\
\text{Output constraints handling: exterior penalty method} \\
\text{Control algorithm: Levenberg-Maquardt’s algorithm}
\]  

(1)
**Stage of development for MPC@CB**

- **History**: created in 2007, under Matlab, with GUI
- **Today**: a standalone application without Matlab is available
The nonlinear model of CSTR

A continuous stirred tank reactor (CSTR): $A \rightarrow B$ is described as follows:

\[
\begin{align*}
\dot{c}_A(t) &= \frac{q}{V}(c_f^A - c_A(t)) - k_0 \exp \left(-\frac{E}{R} \right) / T(t) \right) c_A(t) \\
\dot{T}(t) &= \frac{q}{V}(T_f - T(t)) + \frac{\Delta H}{\rho_c} k_0 \exp \left(-\frac{E}{R} \right) / T(t) \right) c_A + \frac{UA}{\rho V C_p} (T_c - T(t)) \\
y(t) &= c_A(t)
\end{align*}
\]

(Σ)

Where:

- **Input**: the controllable temperature of cooling jacket $T_c(t)$ ($K$).
- **Output**: the concentration of A $c_A(t)$ ($mol/m^3$)
- **Input constraints**: $250K < T_c < 320K$.
- **Output constraint** $y > y_{min} = 0.87$.

**Objective**: use MPC@CB (with or without the output constraint) for the set-point tracking of a reference value 0.86.
Simulation results

- without the output constraint
  - optimal input applied

  ![Graph 1](image1)

  - setpoint trajectory tracking

  ![Graph 2](image2)

  Conclusion: setpoint regulation, OK!

- with the output constraint: $y > y_{\text{min}} = 0.87$
  - optimal input applied

  ![Graph 3](image3)

  - trajectory tracking

  ![Graph 4](image4)

  Conclusion: constrained setpoint regulation, OK!
MPC@CB is easily tunable for any new dynamic process.
The specified user defined constrained control objectives are well achieved by the online closed loop control with MPC@CB.
With the off-line and on-line IMC-MPC structure, the on-line computational time of optimization is decreased by MPC@CB.
More case studies are discussed on the website.
MPC@CB is available: short time evaluation, commercial licence or embedded in a complete turnkey solution for the customer.
References

ODOE4OPE


MPCatCB


Annex A: ODOE4OPE

- **Simulation condition**
  - **Parameters in the model of the bio-reactor**
    
    | Parameter                                                                 | Symbol | Value |
    |---------------------------------------------------------------------------|--------|-------|
    | The maximal specific rate of the biomass \( (h^{-1}) \)                   | \( \mu_{max} \) | 0.3   |
    | The yield \((-)\)                                                         | \( \alpha \)   | 1     |
    | The constant of the saturation \( (g/L) \)                               | \( K \)     | 0.05  |
    | The substrate concentration in the feed \( (g/L) \)                      | \( S_{in} \)  | 2     |

- **Initial conditions and parameters value for the simulation**

    | Initial conditions and Parameters | Symbol |
    |-----------------------------------|--------|
    | Target values of parameters       | \( [\theta_1 \theta_2]_p \) |
    | Initial estimates of parameters   | \( [\hat{\theta}_1(0) \hat{\theta}_2(0)] \) |
    | Initial values of model states    | \( [x_{m1}(0) x_{m2}(0)] \) |
    | Initial estimates of states       | \( [\hat{x}_1(0) \hat{x}_2(0)] \) |
    | Initial estimate of covariance    | \( P(0) \) |
    | Time of the simulation            | \( T_{fin} \) |
    | Sampling period                   | \( T_s \) |
    | Prediction horizon                | \( N_p \) |

Initial values:  
- \( \theta_1(0) = 0.25 \)  
- \( \theta_2(0) = 0.8 \)  
- \( x_{m1}(0) = 0.01 \)  
- \( x_{m2}(0) = 2 \)  
- \( \hat{x}_1(0) = 0.01 \)  
- \( \hat{x}_2(0) = 1.5 \)  
- \( P(0) = 50 \times I \)  
- \( T_{fin} = 100 \)  
- \( T_s = 0.25 \)  
- \( N_p = 8 \)
Observer for bio-reactor

System augmented:

\[
(M) \left\{ \begin{array}{l}
\dot{x}_1(t) = \frac{\theta_1 x_2(t)}{x_2(t) + a_1} x_1(t) - u(t) x_1(t) \\
\dot{x}_2(t) = -\theta_2 \frac{\theta_1 x_2(t)}{x_2(t) + a_1} x_1(t) - u(t) (x_2(t) - a_2) \\
\dot{\theta}_1 = 0 \\
\dot{\theta}_2 = 0 \\
y(t_k) = x_1(t_k),
\end{array} \right.
\]

where \( t_k - t_{k-1} \) is the sampling time measurements.
Extended Kalman Filter (EKF)

<table>
<thead>
<tr>
<th>Model</th>
<th>( \dot{x}(t) = f(x(t), u(t)) + w(t), w(t) \in \mathcal{N}(0, Q(t)) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initialize</td>
<td>( \hat{x}_{0</td>
</tr>
<tr>
<td>Predict</td>
<td>( \begin{cases} \dot{\hat{x}}(t) = f(\hat{x}(t), u(t)) \ \dot{P}(t) = F(t)P(t) + P(t)F(t)^T + Q(t) \end{cases} )</td>
</tr>
<tr>
<td>with</td>
<td>( \begin{cases} \hat{x}(t_{k-1}) = \hat{x}_{k-1</td>
</tr>
<tr>
<td>( \Rightarrow )</td>
<td>( \begin{cases} \hat{x}_{k</td>
</tr>
<tr>
<td>Update</td>
<td>( K_k = P_{k</td>
</tr>
<tr>
<td></td>
<td>( \hat{x}_{k</td>
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<tr>
<td></td>
<td>( P_{k</td>
</tr>
<tr>
<td>where</td>
<td>( F(t) = \left. \frac{\partial f}{\partial x} \right</td>
</tr>
</tbody>
</table>

where 

\[
\dot{x}(t) = f(x(t), u(t)) + w(t), \ w(t) \in \mathcal{N}(0, Q(t))
\]
Annex A: ODOE4OPE

- Sensitivity model of the bio-reactor

\[
\begin{align*}
\dot{x}_{1\theta_1}(t) &= \frac{x_2(t)x_1(t)}{x_2(t) + a_1} - u(t)x_{1\theta_1}(t) + \hat{\theta}_1(t)\frac{x_2(t)x_1\theta_1(t)(x_2(t) + a_1) + a_1x_1(t)x_2\theta_1(t)}{(x_2(t) + a_1)^2} \\
\dot{x}_{1\theta_2}(t) &= -u(t)x_{1\theta_2} + \hat{\theta}_1(t)\frac{x_2(t)x_1\theta_2(t)(x_2(t) + a_1) + a_1x_1(t)x_2\theta_2(t)}{(x_2(t) + a_1)^2} \\
\dot{x}_{2\theta_1}(t) &= -\frac{\hat{\theta}_2(t)x_2(t)x_1(t)}{x_2(t) + a_1} - u(t)x_{2\theta_1}(t) - \hat{\theta}_1(t)\hat{\theta}_2(t)\frac{x_2(t)x_1\theta_1(t)(x_2(t) + a_1) + a_1x_1(t)x_2\theta_1(t)}{(x_2(t) + a_1)^2} \\
\dot{x}_{2\theta_2}(t) &= -\frac{\hat{\theta}_1(t)x_2(t)x_1(t)}{x_2(t) + a_1} - u(t)x_{2\theta_2}(t) - \hat{\theta}_1(t)\hat{\theta}_2(t)\frac{x_2(t)x_1\theta_2(t)(x_2(t) + a_1) + a_1x_1(t)x_2\theta_2(t)}{(x_2(t) + a_1)^2} \\
x_{1\theta_1}(0) &= x_{1\theta_2}(0) = x_{2\theta_1}(0) = x_{2\theta_2}(0) = 0
\end{align*}
\]

(4)

where \( x_{i\theta_j} = \frac{\partial x_i}{\partial \theta_j} \).
The constrained optimization problem based on IMC-MPC structure is described as followed:

\[
\begin{align*}
\min_{\bar{u}} J(\bar{u}) &= \sum_{j \in J_1^{N_p}} g(y_{ref}(j), \Delta y_m(j), \Delta u(j-1), e(k)) \\
\Delta \bar{u} &= [\cdots \Delta u(j) \cdots]^T \quad \forall j \in J_0^{N_c-1} \\
\Delta u(j) &= \Delta u(k + N_c - 1) \quad \forall j \in J_{N_c}^{N_p-1} \\
u_{min} - u_0(j) &\leq \Delta u(j) \leq u_{min} - u_0(j) \quad \forall j \in J_0^{N_p-1} \\
\Delta u_{min} &\leq \Delta u(j) - \Delta u(j-1) \leq \Delta u_{max} \quad \forall j \in J_0^{N_p-1} \\
\Delta u_{min}' &= \Delta u_{min} - (u_0(j) - u_0(j-1)) \quad \forall j \in J_0^{N_p-1} \\
\Delta u_{max}' &= \Delta u_{max} - (u_0(j) - u_0(j-1)) \quad \forall j \in J_0^{N_p-1} \\
c_i(y_{ref}(j), \Delta y_m(j), \Delta u(j-1), e(k)) &\leq 0 \quad \forall j \in J_0^{N_p}, \forall i \in I_1^n \\
\text{and subjet to the resolution of the model } (S_{TVL}).
\end{align*}
\]
### Input constraints handling: hyperbolic transformation:

\[
\begin{align*}
  u(j) &= f(p(j)) = f_{\text{moy}} + f_{\text{amp}} \tanh \left( \frac{p(j) - f_{\text{moy}}}{f_{\text{amp}}} \right) \quad \forall j \in J_0^{N_c-1} \\
  p(j) &\in \mathbb{R} \quad \forall j \in J_0^{N_c-1} \quad \text{(unconstrained input parameter)} \\
  f_{\text{moy}} &= \frac{f_{\text{max}} + f_{\text{min}}}{2} \\
  f_{\text{amp}} &= \frac{f_{\text{max}} - f_{\text{min}}}{2} \\
  f_{\text{min}} &= \max(u_{\text{min}}, u(j - 1) + \Delta u_{\text{min}}) \quad \forall j \in J_0^{N_c-1} \\
  f_{\text{max}} &= \max(u_{\text{max}}, u(j - 1) + \Delta u_{\text{max}}) \quad \forall j \in J_0^{N_c-1}
\end{align*}
\]

(6)

![Fig. Mapping from unconstrained variable \( p \) into constrained variable \( u \)](image_url)
Control algorithm: Levenberg-Maquardt

\[ \Delta \tilde{p}^{n+1} = \Delta \tilde{p}^n - (\nabla^2 J_{tot}^n + \lambda I)^{-1} \nabla J_{tot}^n \] (7)

where the argument \( \Delta \tilde{p} \) is determined at each sample instant \( k \) by this iteration procedure, \( \nabla^2 J_{tot}^n \) and \( \nabla J_{tot}^n \) are the criteria gradient and criteria hessian with respect to \( \Delta \tilde{p}^n \) at the iteration \( n \).