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

Jun QIAN^{1,2}, Pascal DUFOUR^{1,3}, Madiha NADRI¹

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Journée nationale des logiciels de modélisation et de calcul scientifique (LMCS): 07/12/2012





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- For linear and nonlinear dynamic model based systems.

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Closed loop control structure The components Optimal control law design

Closed loop control structure



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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, ...

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Sensitivity model

$$(M_{\theta}) \left\{ \begin{array}{l} \frac{\partial}{\partial t} \tilde{x}_{\theta} = \frac{d}{\partial t} \left(\frac{\partial x}{\partial \theta} \right) = \frac{\partial}{\partial \theta} \left(\frac{\partial x}{\partial t} \right) = \frac{\partial f}{\partial \theta} + \frac{\partial f}{\partial x} \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial \theta} = \tilde{y}_{\theta} = \frac{\partial h}{\partial \theta} + \frac{\partial h}{\partial x} \frac{\partial x}{\partial \theta} \end{array} \right.$$

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(2)

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Optimal control law design

• Sensitivity matrix:

$$Z_{k} = \begin{bmatrix} \frac{\partial x_{1}}{\partial \theta_{1}} \Big|_{k} & \frac{\partial x_{1}}{\partial \theta_{2}} \Big|_{k} & \cdots & \frac{\partial x_{1}}{\partial \theta_{p}} \Big|_{k} \\ \frac{\partial x_{2}}{\partial \theta_{1}} \Big|_{k} & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \vdots \\ \frac{\partial x_{n}}{\partial \theta_{1}} \Big|_{k} & \cdots & \cdots & \frac{\partial x_{n}}{\partial \theta_{p}} \Big|_{k} \end{bmatrix}$$

(3)

- 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 $F(x_{j|k}, u_{j|k}, \theta_{k|k}) = \frac{1}{N_p} \sum_{j=k+1}^{k+N_p} M_{j|k}$
 $c_i(y, x, \theta, u) < 0$ (4)

• Criterion: A-optimality

$$\begin{cases} u = \arg \max_{u \in [u_{min}, u_{max}]} J_A(u) \\ \text{with } J_A(u) = trace(F) \end{cases}$$
(5)

Stage of development

- 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 Simulation results

The nonlinear model of Bio-reactor: $X + S \rightarrow X$

The nonlinear dynamical model of the process is:

$$(\Sigma) \begin{cases} \dot{X}(t) = \frac{\mu_{max}S(t)}{S(t) + K}X(t) - D(t)X(t) \\ \dot{S}(t) = -\alpha \frac{\mu_{max}S(t)}{S(t) + K}X(t) - D(t)(S(t) - S_{in}) \\ y(t) = X(t). \end{cases}$$
(6)

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: μ_{max} and α .
- input constraints: $0 h^{-1} \leq D(j) \leq 0.2 h^{-1}$
- output constraint: $X(j) \leqslant 1.95 \, g/L$

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

Simulation results

The nonlinear model of Bio-reactor Simulation results

• Input applied: D(t)

Simulation results

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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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- 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).
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MPC: general framework

• MPC scheme



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k

k+1 k+2

MPC: general framework

MPC scheme PAST FUTURE **Reference Trajectory** Measured Output Past Control Input Sample Time

...

k+Np

MPC: general framework

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Linearized IMC-MPC structure

Formulation of the optimization problem solved in a MPC approach

Linearized IMC-MPC structure



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.

Linearized IMC-MPC structure Formulation of the optimization problem solved in a MPC approach

Formulation of the optimization problem solved in a MPC approach

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

(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 Simulation results

The nonlinear model of CSTR

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

$$(\Sigma) \begin{cases} \dot{c}_{A}(t) = \frac{q}{V}(c_{A}^{f} - c_{A}(t)) - k_{0}exp\left(-\left(\frac{E}{R}\right)/T(t)\right)c_{A}(t) \\ \dot{T}(t) = \frac{q}{V}(T_{f} - T(t)) + \frac{\Delta H}{\rho C_{\rho}}k_{0}exp\left(-\left(\frac{E}{R}\right)/T(t)\right)c_{A} + \frac{UA}{\rho V C_{\rho}}(T_{c} - T(t)) \\ y(t) = c_{A}(t) \end{cases}$$

$$(2)$$

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.

The nonlinear model of CSTR Simulation results

Simulation results

- without the output constraint
 - optimal input applied



setpoint trajectory tracking



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Conclusion: setpoint regulation, OK!

• with the output constraint: $y > y_{min} = 0.87$

optimal input applied



trajectory tracking



Conclusion: constrained setpoint regulation, OK!

Conclusion

- 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.

Contact for the softwares

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MPC@CB

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Annex A: ODOE40PE

Simulation condition

• Parameters in the model of the bio-reactor

Parameter	Symbol	Value
The maximal specific rate of the biomass (h^{-1})	μ_{max}	0.3
The yield (-)	α	1
The constant of the saturation (g/L)	K	0.05
The substrate concentration in the feed (g/L)	Sin	2

• Initial conditions and parameters value for the simulation

Initial conditions and Parameters	Symbol	Value (Unit)
Target values of parameters	$[\theta_1 \theta_2]_p$	[0.3 1]
Initial estimates of parameters	$[\hat{ heta}_1(0)\hat{ heta}_2(0)]$	[0.25 0.8]
Initial values of model states	$[x_{m1}(0) x_{m2}(0)]$	[0.01 2]
Initial estimates of states	$[\hat{x}_1(0) \hat{x}_2(0)]$	[0.01 1.5]
Initial estimate of covariance	P(0)	50 imes I
Time of the simulation	T _{fin}	100 h
Sampling period	Ts	0.25 h
Prediction horizon	Np	8

Annex A: ODOE4OPE

- Observer for bio-reactor
 - System augmented:

$$(M) \begin{cases} \dot{x}_{1}(t) = \frac{\theta_{1}x_{2}(t)}{x_{2}(t) + a_{1}}x_{1}(t) - u(t)x_{1}(t) \\ \dot{x}_{2}(t) = -\theta_{2}\frac{\theta_{1}x_{2}(t)}{x_{2}(t) + a_{1}}x_{1}(t) - u(t)(x_{2}(t) - a_{2}) \\ \dot{\theta}_{1} = 0 \\ \dot{\theta}_{2} = 0 \\ y(t_{k}) = x_{1}(t_{k}), \end{cases}$$
(3)

where $t_k - t_{k-1}$ is the sampling time measurements.

Annex A: ODOE4OPE

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• Extended Kalman Filter (EKF)

$$\begin{array}{lll} \mbox{Model} & \dot{x}(t) = f(x(t), u(t)) + w(t), w(t) \in N(0, Q(t)) \\ & y_k = h(x_k) + v_k, v_k \in N(0, R_k) \mbox{ where } x_k = x(t_k) \\ \mbox{Initialize} & \hat{x}_{0|0} = E[x(t_0)], P_{0|0} = Var[x(t_0)] \\ \mbox{Predict} & \begin{cases} \dot{\hat{x}}(t) = f(\hat{x}(t), u(t)) \\ \dot{\hat{P}}(t) = F(t)P(t) + P(t)F(t)^T + Q(t) \\ & with \begin{cases} \dot{\hat{x}}(t_{k-1}) = \hat{x}_{k-1|k-1} \\ P(t_{k-1}) = P_{k-1|k-1} \\ \end{pmatrix} \\ & \begin{cases} \dot{\hat{x}}_{k|k-1} = \hat{x}(t_k) \\ P_{k|k-1} = P(t_k) \\ \end{pmatrix} \\ \mbox{Update} & K_k = P_{k|k-1}H_k^T(H_kP_{k|k-1}H_k^T + R_k)^{-1} \\ & \hat{\hat{x}}_{k|k} = \hat{\hat{x}}_{k|k-1} + K_k(y_k - h(\hat{\hat{x}}_{k|k-1})) \\ P_{k|k} = (I - K_kH_k)P_{k|k-1} \\ & where F(t) = \frac{\partial f}{\partial x}\Big|_{\hat{x}(t),u(t)}, \ H(t) = \frac{\partial h}{\partial x}\Big|_{\hat{x}_{k|k-1}} \end{array}$$

Annex A: ODOE4OPE

• Sensitivity model of the bio-reactor

$$\begin{cases} \dot{x}_{1\theta1}(t) = \frac{x_2(t)x_1(t)}{x_2(t) + a_1} - u(t)x_{1\theta1}(t) + \hat{\theta}_1(t)\frac{x_2(t)x_{1\theta1}(t)(x_2(t) + a_1) + a_1x_1(t)x_{2\theta1}(t)}{(x_2(t) + a_1)^2} \\ \dot{x}_{1\theta2}(t) = -u(t)x_{1\theta2} + \hat{\theta}_1(t)\frac{x_2(t)x_{1\theta2}(t)(x_2(t) + a_1) + a_1x_1(t)x_{2\theta2}(t)}{(x_2(t) + a_1)^2} \\ \dot{x}_{2\theta1}(t) = -\frac{\hat{\theta}_2(t)x_2(t)x_1(t)}{x_2(t) + a_1} - u(t)x_{2\theta1}(t) - \hat{\theta}_1(t)\hat{\theta}_2(t)\frac{x_2(t)x_{1\theta1}(t)(x_2(t) + a_1) + a_1x_1(t)x_{2\theta1}(t)}{(x_2(t) + a_1)^2} \\ \dot{x}_{2\theta2}(t) = -\frac{\hat{\theta}_1(t)x_2(t)x_1(t)}{x_2(t) + a_1} - u(t)x_{2\theta2}(t) - \hat{\theta}_1(t)\hat{\theta}_2(t)\frac{x_2(t)x_{1\theta2}(t)(x_2(t) + a_1) + a_1x_1(t)x_{2\theta2}(t)}{(x_2(t) + a_1)^2} \\ \dot{x}_{1\theta1}(0) = x_{1\theta2}(0) = x_{2\theta1}(0) = x_{2\theta2}(0) = 0 \end{cases}$$
(4)
where $x_{i\theta_j} = \frac{\partial x_i}{\partial \theta_j}$.

Annex B: MPC@CB

• The constrained optimization problem based on IMC-MPC structure is described as followed:

$$\min_{\tilde{u}} J(\tilde{u}) = \sum_{j \in \mathcal{J}_{1}^{N_{p}}} g(y_{ref}(j), \Delta y_{m}(j), \Delta u(j-1), e(k))$$

$$\Delta \tilde{u} = [\cdots \Delta u(j) \cdots]^{T} \quad \forall j \in \mathcal{J}_{0}^{N_{p}-1}$$

$$\Delta u(j) = \Delta u(k + N_{c} - 1) \quad \forall j \in \mathcal{J}_{N_{c}}^{N_{p}-1}$$

$$u_{min} - u_{0}(j) \leq \Delta u(j) \leq u_{min} - u_{0}(j) \quad \forall j \in \mathcal{J}_{0}^{N_{p}-1}$$

$$\Delta u_{min}^{'} \leq \Delta u(j) - \Delta u(j-1) \leq \Delta u_{max}^{'} \quad \forall j \in \mathcal{J}_{0}^{N_{p}-1}$$

$$\Delta u_{min}^{'} = \Delta u_{min} - (u_{0}(j) - u_{0}(j-1)) \quad \forall j \in \mathcal{J}_{0}^{N_{p}-1}$$

$$\Delta u_{max}^{'} = \Delta u_{max} - (u_{0}(j) - u_{0}(j-1)) \quad \forall j \in \mathcal{J}_{0}^{N_{p}-1}$$

$$c_{i}(y_{ref}(j), \Delta y_{m}(j), \Delta u(j-1), e(k)) \leq 0 \quad \forall j \in \mathcal{J}_{0}^{N_{p}}, \quad \forall i \in \mathcal{I}_{1}^{n}$$
and subjet to the resolution of the model $(S_{TVL}).$

Annex B: MPC@CB

• Input constraints handling: hyperbolic transformation:

$$u(j) = f(p(j)) = f_{moy} + f_{amp} tanh(\frac{p(j) - f_{moy}}{f - amp}) \quad \forall j \in \mathcal{J}_0^{N_c - 1}$$

$$p(j) \in \mathbb{R} \; \forall j \in \mathcal{J}_0^{N_c - 1} \text{ (unconstrained input parameter)}$$

$$f_{moy} = \frac{f_{max} + f_{min}}{2}$$

$$f_{amp} = \frac{f_{max} - f_{min}}{2}$$

$$f_{min} = \max(u_{min}, u(j - 1) + \Delta u_{min}) \quad \forall j \in \mathcal{J}_0^{N_c - 1}$$

$$f_{max} = \max(u_{max}, u(j - 1) + \Delta u_{max}) \quad \forall j \in \mathcal{J}_0^{N_c - 1}$$
(6)



Fig. Mapping from unconstrained variable p into constrained variable u



• 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 $\Delta \tilde{\rho}$ is determined at each sample instant k by this iteration procedure, $\nabla^2 J_{tot}^n$ and ∇J_{tot}^n are the criteria gradient and criteria hessain with respect to $\Delta \tilde{\rho}^n$ at the iteration *n*.