



Model-based Control and Optimization with Imperfect Models

Weihua Gao, Simon Wenzel, Sergio Lucia, Sankaranarayanan Subramanian, Sebastian Engell

Process Dynamics and Operations Group Dept. of Biochemical and Chemical Engineering, TU Dortmund, Germany







The Dortmund Process Dynamics and Operations Group





- about 25 PhD candidates from many countries, having degrees in (Bio-)Chemical Engineering, Computer Science, Electrical Engineering, Automation and Robotics ...
- 5 PostDocs: Weihua Gao, Radoslav Paulen, Maren Urselmann, Jian Cui, Elrashid Idris
- 2 part-time secretaries, 1 technician
- More than 65 finished PhD theses since 1990

Outline

- Motivation
- Iterative optimization using modifier adaptation
- Multi-stage optimizing control
 - Idea and problem formulation
 - Results for a case study
 - Output feedback multi-stage optimizing control
- Summary





Motivation for optimizing control

Operational excellence

- Optimal utilization of equipment and resources
- Minimization of unplanned shut-downs
- Meeting of quality standards without re-work
- Energy efficiency
- Resource efficiency
- Operations in the process industries are subject to significant uncertainties
 - Changing process behaviours (e.g. catalyst efficiency)
 - Changing equipment
 - Changing feeds
 - External influences as e.g. outside temperature

Efficient, safe and reliable operation requires reactive measurement-based control and optimization

U technische universität dortmund



Available technologies

Feedback control to track given set-points and constraints

- Requires a margin around the constraints
- Set-points must be chosen well
- Optimization of the set-points and feedback control (Real-time Optimization (RTO) plus classical control or MPC)
- Model-based (directly) optimizing control:
 - The target of the controller is an economic optimization under constraints:
 - Safety limits
 - Product quality constraints
 - Equipment limitations

S. Engell: Feedback Control for Optimal Process Operation. J. Process Control 17, 2007, 203-219

RTO and optimizing control depend critically on the accuracy of the model that is employed.





Focus of this talk

- In this talk the focus is on optimization and control using inaccurate or simplified models.
- New strategies for robust control and optimization will be presented:
 - MAwQA Modifier Adaptation with Quadratic Approximation Robust iterative data and model based optimization
 - MSNMPC Multi-stage Nonlinear Model Predictive Control
 A new efficient robust NMPC strategy







Department of Biochemical and Chemical Engineering Process Dynamics and Operations Group (DYN)

Iterative Optimizing Control by Modifier Adaptation with Quadratic Approximation

Weihua Gao, Simon Wenzel, Sebastian Engell



The research leading to these results was funded by the ERC Advanced Investigator Grant MOBOCON under the grant agreement No. 291458.



Real-time optimization



- Model-based upper-level optimization system
- Quasi-stationary optimization of the set-points of the plant
- Targeting economic optimality



Optimization and control with imperfect models Lyngby, May 31, 2016



Batch chromatography



technische universität dortmund



General Rate Model





Optimization and control with imperfect models Lyngby, May 31, 2016 D



Effect of uncertainty in the adsorption isotherm



Challenge: Optimization in the presence of model uncertainty



Optimization and control with imperfect models Lyngby, May 31, 2016



Measurement-based RTO strategies





Optimization and control with imperfect models Lyngby, May 31, 2016



The principle of Modifier Adaptation

Using the collected data, the bias (offset) between the plant and the model and the empirical gradients are estimated and used to modify the optimization problem:

Instead of

$$\min_{\mathbf{u}} \quad J_m(\mathbf{u})$$
 s.t. $\mathbf{C}_m(\mathbf{u}) \le \mathbf{0}$

the optimizer solves

$$\begin{split} \min_{\mathbf{u}} & J_{ad}^{(k)}(\mathbf{u}) = J_m(\mathbf{u}) + J_p^{(k)} - J_m^{(k)} + \left(\nabla J_p^{(k)} - \nabla J_m^{(k)}\right)^T \left(\mathbf{u} - \mathbf{u}^{(k)}\right) \\ \text{s.t.} & \mathbf{C}_{ad}^{(k)}(\mathbf{u}) = \mathbf{C}_m(\mathbf{u}) + \mathbf{C}_p^{(k)} - \mathbf{C}_m^{(k)} + \left(\nabla \mathbf{C}_p^{(k)} - \nabla \mathbf{C}_m^{(k)}\right)^T \left(\mathbf{u} - \mathbf{u}^{(k)}\right) \leq \mathbf{0} \\ \end{split}$$
bias modifiers

If the bias and gradients are correct, this converges to the true optimum!



Optimization and control with imperfect models Lyngby, May 31, 2016



Gradient estimation

Finite difference approximation from the measurements at the latest n_u +1 setpoints:

$$\mathbf{S}^{(k)} = \left[\left(\mathbf{u}^{(k)} - \mathbf{u}^{(k-1)} \right) \cdots \left(\mathbf{u}^{(k)} - \mathbf{u}^{(k-n_u)} \right) \right]^T$$

$$\nabla J_p^{(k)} = \left[\mathbf{S}^{(k)}\right]^{-1} \cdot \left[\left(J_p^{(k)} - J_p^{(k-1)} \right) \cdots \left(J_p^{(k)} - J_p^{(k-n_u)} \right) \right]^T$$

S can become ill-conditioned \rightarrow gradient becomes unreliable

- Monitoring of the condition number
- Additional moves to improve the condition number
 W. Gao and S. Engell: Iterative Set-Point Optimization of Batch Chromatography, Computers and Chemical Engineering 29, 2005, 1401 - 1410
- Setpoints close to each other: Approximation good but sensitive to noise
- Setpoints far apart: Error in the gradient but robust

J technische universität dortmund



Influence of noise on the gradient error





U technische universität dortmund

Optimization and control with imperfect models Lyngby, May 31, 2016

15

Process Dynamics and Operations

Quadratic approximation in Derivative-free Optimization

Optimization and control with imperfect models

Lyngby, May 31, 2016

- Optimization based upon probing of the target function
- Repeatedly constructing local quadratic functions

$$\min_{\mathcal{P}} \sum_{i=1}^{n_r} \left(J_p\left(\mathbf{u}^{(r_i)}\right) - J_\phi\left(\mathbf{u}^{(r_i)}, \mathcal{P}\right) \right)^2$$
$$J_\phi\left(\mathbf{u}, \mathcal{P}\right) = \sum_{i=1}^{n_u} \sum_{j=1}^i a_{i,j} u_i u_j + \sum_{i=1}^{n_u} b_i u_i + c$$

 Mathematically well founded

Idea: Estimate the gradients via quadratic approximation

technische universität

dortmund

50 45 40 35 30 25 20 15 0 10 5-2 0 3 3 2.5 2 1.5 0.5 0 -0.5 -1.5 -2



MAWQA-Algorithm

- Modifier Adaptation with Quadratic Approximation
- Iterative optimization combined with estimation of the gradients by quadratic approximation
- Theory available how to choose the points which are interpolated to get a good approximation of the curvature
 - Nearby points for accuracy
 - Distant points for robustness
- Trust region estimation prevents too large steps
- Monitoring of model quality and switching between MA and pure DFO

Weihua Gao, Simon Wenzel and Sebastian Engell IFAC ADCHEM 2015 European Control Conference 2015 Computers and Chemical Engineering, online 2016





Gradient computed by quadratic approximation



dortmund



Lyngby, May 31, 2016

Process Dynamics and Operations

Gradient via quadratic approximation

- Capture the curvature information from more distant points to decrease the approximation error
- Explore the inherent smoothness of the mapping to decrease the influence of the noise



Screen points for a well-distributed regression set







Illustration of regression set screening

Optimization and control with imperfect models

Lyngby, May 31, 2016



 \odot local points, \odot chosen outer points, \bigcirc unchosen points.

technische universität

dortmund

 $\mathcal{U}^{(k)} = \mathcal{U}_{nb} \cup \mathcal{U}_{dist}$

 \mathcal{U}_{nb} are determined by

$$\mathcal{U}_{nb} = \{\mathbf{u} : \|\mathbf{u} - \mathbf{u}^{(k)}\| \le \Delta \mathbf{u}; \mathbf{u} \in \mathbb{U}\}$$

 \mathcal{U}_{dist} are determined by

$$\min_{\mathcal{U}_{dist}} \quad \frac{\sum_{\mathbf{u} \in \mathcal{U}_{dist}} \|\mathbf{u} - \mathbf{u}^{(k)}\|}{\varphi(\mathcal{U}_{dist})}$$
s.t. size(\mathcal{U}_{dist}) = $(n_u + 1)(n_u + 2)/2 - 1$
 $\mathcal{U}_{dist} \subset \mathbb{U} \setminus \mathcal{U}_{nb}$

Sufficiently distant and well-distributed points are indispensable for capturing the curvature reliably from noisy data

The use of many points in a neighborhood can improve the accuracy of the gradient estimation



Trust region



$$\mathcal{B}^{(k)} : (\mathbf{u} - \mathbf{u}^{(k)})^T M^{-1} (\mathbf{u} - \mathbf{u}^{(k)}) \le \gamma^2$$
$$M = cov(\mathcal{U}^{(k)})$$

- Allow large moves along a direction in which more data has been collected
- Bound aggressive moves along a direction in which the plant still needs to be probed



Optimization and control with imperfect models Lyngby, May 31, 2016



Application to the batch chromatography example



Significantly improved robustness to noise and speed of convergence compared to our previous work (and to that of others).



Optimization and control with imperfect models Lyngby, May 31, 2016



Ten-variable synthetic example

$$\begin{array}{ll} \min_{\mathbf{x}} & f(x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}) \\ \text{s.t.} & -105 + 4x_1 + 5x_2 - 3x_7 + 9x_8 \leq 0 \\ & 10x_1 - 8x_2 - 17x_7 + 2x_8 \leq 0 \\ & -8x_1 + 2x_2 + 5x_9 - 2x_{10} - 12 \leq 0 \\ \hline z(x_1, x_2, x_3, x_4) \leq 0 \\ & 5x_1^2 + 8x_2 + (x_3 - 6)^2 - 2x_4 - 40 \leq 0 \\ & x_1^2 + 2(x_2 - 2)^2 - 2x_1x_2 + 14x_5 - 6x_6 \leq 0 \\ & 0.5(x_1 - 8)^2 + 2(x_2 - 4)^2 + 3x_5^2 - x_6 - 30 \leq 0 \\ & -3x_1 + 6x_2 + 12(x_9 - 8)^2 - 7x_{10} \leq 0 \\ & 0 \leq x_i \leq 10, \quad i = 1, \dots, 10. \end{array}$$

Caballero and Grossmann (2008): Algorithm based on fitting response surface takes 800 sampled points to reach the optimum.

Process Dynamics and Operations

Optimization results for the synthetic example



Generation of data-collecting moves

- The regression set is not well-poised
- In the probed operating range, the function is not quadratic



Dual-control mechanism with set-point moves









Department of Biochemical and Chemical Engineering Process Dynamics and Operations Group (DYN)

Multi-stage Nonlinear Model-predictive Control

Sergio Lucia, Sankaranarayanan Subramanian, Sebastian Engell



The research leading to these results was supported by the German Research Council DFG



The research leading to these results was supported by the ERC Advanced Investigator Grant MOBOCON under the grant agreement No. 291458.



Model predictive control



dortmund

MPC

- Solve optimization problem
 - Mathematical Model
 - Cost function
 - Constraints
- Apply first control input
 - Take new measurements
- Optimize again
- Apply first control input
- Take new measurements and optimize again
- Economic cost function can be used in the optimization \rightarrow optimizing control





Model predictive control: Wrong model





Optimization and control with imperfect models Lyngby, May 31, 2016



Multi-stage NMPC: Formulation



- Uncertainty is modelled by a scenario tree
- Constraints must be met for all values of the uncertainty
- Controller can react to the information gained at the next stage
- This is taken into account in the optimization of the next decisions

J technische universität dortmund

Optimization and control with imperfect models Lyngby, May 31, 2016

29

Process Dynamics and Operations

Robust Multi-Stage NMPC

- Closed-loop formulation by means of an open loop optimization problem
 - Applied to scheduling problems [Sand and Engell, Comp. Chem. Engg. 2005]
 - Early work on linear MPC [de la Peña et al., 2005], [Bernardini et al., 2009]
- Proposed for Nonlinear MPC in [Dadhe & Engell, 2008]
- Many publications by [Lucia et al.] since 2012 with promising results, [Lucia, Finkler, Engell, ADCHEM 2012, J. Proc. Control 2013, …]





and Operations

Multi-stage NMPC: Robust horizon

 Avoid the exponential growth by branching the tree only up to the robust horizon









An industrial batch polymerization reactor control problem



S. Lucia, J. Andersson, H. Brandt, M. Diehl, S. Engell: Handling Uncertainty in Economic Nonlinear Model Predictive Control, J. Process Control 24 (2014), 1247-1259



Optimization and control with imperfect models Lyngby, May 31, 2016



Industrial batch polymerization reactor model

$$\begin{split} \dot{m}_{W} &= \dot{m}_{W,F} & \text{8 differential states} \\ \dot{m}_{A} &= \dot{m}_{A,F} - k_{R1} m_{A,R} - \frac{p_{1} k_{R2} m_{AWT} m_{A}}{m_{ges}} & \text{3 control inputs} \\ \dot{m}_{P} &= k_{R1} m_{A,R} + \frac{p_{1} k_{R2} m_{AWT} m_{A}}{m_{ges}} & \text{2 uncertain parameters} \\ \dot{T}_{R} &= \frac{1}{c_{p,R} m_{ges}} \begin{bmatrix} \dot{m}_{F} c_{p,F} (T_{F} - T_{R}) + \Delta H_{R} k_{R1} m_{A,R} - k_{K} A (T_{R} - T_{S}) - \dot{m}_{AWT} c_{p,R} (T_{R} - T_{EK}) \end{bmatrix} \\ \dot{T}_{S} &= 1/(c_{p,S} m_{S}) [k_{K} A (T_{R} - T_{S}) - k_{K} A (T_{S} - T_{M})] \\ \dot{T}_{M} &= \frac{1}{c_{p,W} m_{M,KW}} [\dot{m}_{M,KW} c_{p,W} (T_{M}^{TN} - T_{M}) + k_{K} A (T_{S} - T_{M})] \\ \dot{T}_{EK} &= \frac{1}{c_{p,R} m_{AWT}} \left[\dot{m}_{AWT} c_{p,W} (T_{R} - T_{EK}) - \alpha (T_{EK} - T_{AWT}) + \frac{p_{1} k_{R2} m_{A} m_{AWT} \Delta H_{R}}{m_{ges}} \right] \\ \dot{T}_{AWT} &= \frac{1}{c_{p,W} m_{AWT,KW}} \left[\dot{m}_{AWT,KW} c_{p,W} (T_{AWT}^{TN} - T_{AWT}) - \alpha (T_{AWT} - T_{EK}) \right] \\ k_{R1} &= k_{0} e^{-\frac{E_{a}}{RT_{R}}} (k_{U1} (1 - U) + k_{U2} U) \\ k_{R2} &= k_{0} e^{-\frac{E_{a}}{RT_{EK}}} (k_{U1} (1 - U) + k_{U2} U) \\ \end{split}$$

J technische universität dortmund

Optimization and control with imperfect models Lyngby, May 31, 2016 33

Process Dynamics and Operations

Control task:

- Minimize the batch time while satisfying temperature constraints for all values of two uncertain (±30 %) parameters
- Standard NMPC with tracking cost:

$$J_{\text{track}} = \sum_{k=0}^{N_p - 1} -m_{P,k}^j + q \left(T_{R,k}^j - T_{\text{set}}\right)^2 + r \Delta u_k^j^2$$

• Multi-stage NMPC with economic cost function: $J_{eco} = \sum_{i=1}^{N} \omega_i \sum_{k=0}^{N_p-1} -m_{P,k}^j + r \Delta u_k^j^2$



Optimization and control with imperfect models Lyngby, May 31, 2016



Standard NMPC: No uncertainties

Comparison of tracking and economic NMPC





Optimization and control with imperfect models Lyngby, May 31, 2016



Simulation results for different scenarios



Simulations for different values of k and ΔH (±30%)



Optimization and control with imperfect models Lyngby, May 31, 2016



Simulation results for different scenarios

Multi-stage NMPC

- Simple scenario tree
 - 3 extreme values of the uncertainties
 - Tree branches only at the fist stage







Optimization and control with imperfect models Lyngby, May 31, 2016



Comparison with standard NMPC

Scenario		Batch time in hours		
ΔH_R	k_0	Standard NMPC	Standard (cons.)	Multi-stage
+30%	+30%	infeasible	2.15	2.03
+30%	0%	infeasible	2.72	2.24
+30%	-30%	infeasible	4.05	2.69
0%	+30%	1.60	2.22	1.60
0%	0%	1.81	3.00	1.84
0%	-30%	2.69	4.57	2.50
-30%	+30%	1.50	2.72	1.43
-30%	0%	1.99	3.57	1.86
-30%	-30%	2.88	5.11	2.68
Av. batch t	ime [h]	infeasible	3.35	2.10

Batch time reduction of 60% w.r.t. standard (cons.) NMPC

Comp time [s]	Standard NMPC	Standard (cons.)	Multi-stage
Average	0.072	0.059	1.134
Maximum	0.230	0.179	1.550



Optimization and control with imperfect models Lyngby, May 31, 2016



Comparison with open-loop robust NMPC





Optimization and control with imperfect models Lyngby, May 31, 2016



Output feedback NMPC - Motivation



 The values of the states are not known generally. The states need to be estimated based on measurements.

U technische universität dortmund



Multi-stage output feedback NMPC

Instead of predicting the future state, predict the estimates

 $\hat{x}_{k+1} = f_{est}(\hat{x}_k, u_k, d_k)$

 If the estimates can be predicted, the states can be assumed to be bounded by

 $x_k \in \hat{x}_k \oplus \Sigma_k$

- Since we know the estimates at every time, the feedback policy can be obtained based on the predicted estimates
- EKF or UKF equations can be used to get

 $\hat{x}_{k+1} = f(\hat{x}_k, u_k, d_k) + K_k \nu_k$





Multi-stage output feedback NMPC using the EKF

- Start with current estimate \hat{x}_0 and covariance information P_0 from the estimator
- Propagate the state estimate and the covariance information
- Use the EKF equations to estimate future states for different values of the innovations

•
$$\hat{x}_{k+1} = f(\hat{x}_k, u_k, p_k) + K_k v_k$$

• The covariance of the innovations $(C_k P_k^- C_k^T + R_k)$ is used to get the samples of the innovations





Output feedback NMPC – Problem formulation

Mathematical formulation:

$$\begin{split} \min_{u_k^j} \sum_{i=1}^N \omega_i \, J_i \\ J_i &= \sum_{k=0}^{N_p - 1} L(\hat{x}_{k+1}^j, u_k^j), \forall \hat{x}_{k+1}^j, u_k^j \in S_i \quad \begin{array}{l} \text{Kalman update} \\ \text{with the sampled} \\ \text{innovations} \\ \hat{x}_{k+1}^j &= f\left(\hat{x}_k^{p(j)}, u_k^j, d_k^{r(j)}\right) + K_k^j v_k^{r(j)} \quad \forall (j, k+1) \in I \\ K_k^j &= \Phi\left(\hat{x}_k^{p(j)}, u_k^j, d_k^{r(j)}, P_k^{p(j)}\right) \quad \begin{array}{l} \text{The EKF/ UKF} \\ \text{equations} \\ \forall (j, k) \in I \\ \forall (j, k) \in I \\ \{\hat{x}_k^j\} \bigoplus \{\sigma_k^j\} \in \mathbb{X}, \quad u_k^j \in \mathbb{U} \quad \forall (j, k) \in I \\ u_k^j &= u_k^l \text{ if } x_k^{p(j)} = x_k^{p(l)} \quad \forall (j, k) \in I \\ \end{array}$$

technische universität dortmund



Industrial batch polymerization reactor

$$\begin{split} \dot{m}_{W} &= \dot{m}_{W,F} \\ \dot{m}_{A} &= \dot{m}_{A,F} - \frac{k_{R1}}{k_{R1}} m_{A,R} - \frac{p_{1}k_{R2}}{m_{ges}} m_{AWT} m_{A} \\ \dot{m}_{ges} \\ \dot{m}_{P} &= \frac{k_{R1}}{k_{R1}} m_{A,R} + \frac{p_{1}k_{R2}m_{AWT}m_{A}}{m_{ges}} \\ \dot{T}_{R} &= \frac{1}{c_{p,R}m_{ges}} \left[\frac{m_{F}}{m_{F}}c_{p,F}(T_{F} - T_{R}) + \Delta H_{R}k_{R} m_{A,R} - k_{K}A(T_{R} - T_{S}) - \dot{m}_{AWT}c_{p,R}(T_{R} - T_{EK}) \right] \\ \dot{T}_{S} &= 1/(c_{p,S}m_{S})[k_{K}A(T_{R} - T_{S}) - k_{K}A(T_{S} - T_{M})] \\ \dot{T}_{M} &= \frac{1}{c_{p,W}m_{M,KW}} \left[\dot{m}_{M,KW}c_{p,W}(T_{M}^{IN} - T_{M}) + k_{K}A(T_{S} - T_{M}) \right] \\ \dot{T}_{EK} &= \frac{1}{c_{p,R}m_{AWT}} \left[\dot{m}_{AWT}c_{p,W}(T_{R} - T_{EK}) - \alpha(T_{EK} - T_{AWT}) + \frac{p_{1}k_{R2}m_{A}m_{AWT}\Delta H_{R}}{m_{ges}} \right] \\ \dot{T}_{AWT} &= \frac{1}{c_{p,W}m_{AWT,KW}} \left[\dot{m}_{AWT}c_{p,W}(T_{R} - T_{EK}) - \alpha(T_{EK} - T_{AWT}) - \alpha(T_{AWT} - T_{EK}) \right] \\ k_{R1} &= k_{0}e^{-\frac{E_{A}}{RT_{R}}} (k_{U1}(1 - U) + k_{U2}U) \\ k_{R2} &= k_{0}e^{-\frac{E_{A}}{RT_{EK}}} (k_{U1}(1 - U) + k_{U2}U) \\ \end{split}$$

U technische universität dortmund



- Control task:
 - Minimize the batch time while satisfying temperature constraints for all the values of the uncertainty (±30 %)
 - Constraint on the temperature of the reactor (90±2) $^{\circ}$ C
- Economic cost function

$$J_{\text{eco}} = \sum_{i=1}^{N} \omega_i \sum_{k=0}^{K-1} -m_{P,k}^j + r_1 \Delta \dot{m}_{F,k}^j + r_2 \Delta T_{M,k}^{IN,j} + r_3 \Delta T_{AWT,k}^{IN,j}$$

- Only the measurements of 2 states T_R and T_M are available with measurement noise, standard deviation $\sigma = 0.3$ K
- EKF with parameter estimation is used
- Prediction horizon = 10 samples
- Robust horizon = 1 sample
- Sampling time = 90 s



Standard vs output feedback scheme



 $k_0^{true} = 1.3 k_0^{nom}$





Multi-stage optimizing control - Conclusions

- The improvement of the robustness is very convincing.
- Direct solution without a need for specific engineering
- Improvement over nominal NMPC even when parameter updates are available online

S. Lucia, T. Finkler, S. Engell: Multi-Stage nonlinear model predictive control applied to a semi-batch polymerization reactor under uncertainty, *J. Process Control* 23, 2013, 1306-1319

■ Numerically tractable → DO MPC based upon CasADi

There is more:

- Multiple model state estimation to update the probabilities in the scenario tree
- Dual control improving the model accuracy to improve the control performance
- Guaranteed constraint satisfaction by reachability analsis also for values that are not in the scenario tree

U technische universität dortmund



Summary

- Advanced control offers a significant potential for improved operations!
- One can control well with inaccurate models!
- Two solutions presented:
 - Iterative model **and** data based optimization
 - Multi-stage robust model-based optimization
- Modeling effort is the bottleneck in the solution of practical problems.
 - Robust optimization and control reduce the modeling effort!
- Difficult problem: Satisfaction of complex product property constraints
 - Soft sensors and additional online measurements not necessarily selective, e.g. ultrasound, conductivity, pH, turbidity
 - Online measurements, e.g. NIR or Raman spectroscopy
- Open-source software for efficient implementation of NMPC and MS-NMPC: DO-MPC







Department of Biochemical and Chemical Engineering Process Dynamics and Operations Group (DYN)

Thank you very much for your attention!

Sponsored by:



The research leading to these results was supported by the German Research Council DFG



The research leading to these results was supported by the ERC Advanced Investigator Grant MOBOCON under the grant agreement No. 291458.

