Nonlinear Measurement Combinations for Optimal Operation

Johannes Jäschke, Sigurd Skogestad

Norwegian University of Science and Technology (NTNU)
Trondheim

NTNU
Innovation and Creativity

Outline

Optimizing Control Concepts

On-line Optimization - Conventional RTO

- Optimal operation achieved by using measurements to update a process model at given sample times
- On-line optimization of the model, computed inputs are implemented

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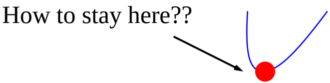
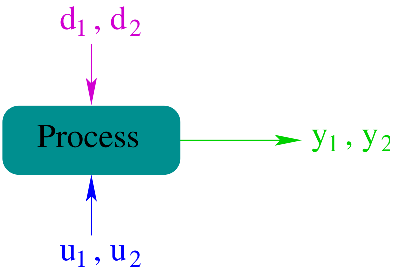
Off-line Optimization - Explicit RTO



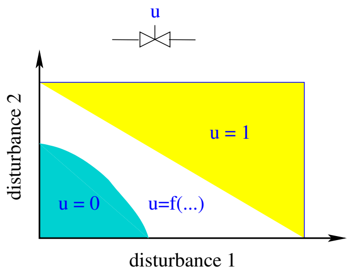
- Precomputed solutions
- For each set of active constraints find optimally invariant variable combinations
- These variables can be be controlled by simple PID controllers
- No need for expensive real-time computations

Motivating example

General Process



Optimal Operating Regions



Motivating example

- Process objective: $\min f(u,d) = \min u_1(u_1 - 2d_2) + u_2(u_2 - 2d_1)$
- Inputs: u_1, u_2, Disturbances: d_1, d_2

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With measurements:

- $y_1 = \frac{2}{u_1 d_1}(d_2 - d_1^2 - 1)$ and $y_2 = \frac{1}{u_1}(d_1 - 1)$

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With measurements:

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- $c_{s,1}^y = -u_1^2 y_1 y_2 + 2u_1^2 y_2^2 - u_1 y_1 + 4u_1 y_2 + 2u_1 = 0$
- $c_{s,2}^y = -2u_1 y_2 + 2u_2 - 2 = 0$

Explicit RTO procedure

1. Formulate the optimization problem:
   min $f(\mathbf{u}, \mathbf{x}, \mathbf{d})$ s.t. $g(\mathbf{u}, \mathbf{x}, \mathbf{d}) \leq 0$ and $h(\mathbf{u}, \mathbf{x}, \mathbf{d}) = 0$
2. Identify the regions of constant active constraints in the disturbance space
3. For each region determine invariant variable combinations
4. Eliminate unknown variables in invariants by measurement relations
5. In each region
   - control the active constraints
   - control invariant measurement combinations $\mathbf{c}_s^y = f(\mathbf{y})$
6. Implement a logic to change regions

Modified Null-space method – Linear Case (based on [1])

Theorem (Quadratic objective, linear constraints)

Consider the optimization problem:

$$\min [\mathbf{z}^T\, \mathbf{d}^T] \begin{bmatrix} \mathbf{J_{zz}} & \mathbf{J_{zd}} \\ \mathbf{J_{zd}}^T & \mathbf{J_{dd}} \end{bmatrix} \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix}$$

subject to:

$$\mathbf{A}_z\mathbf{z} + \mathbf{A}_d\mathbf{d} = \tilde{\mathbf{A}} \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix} = \mathbf{b}$$

$$\mathbf{y} = \tilde{\mathbf{G}}^y \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix}$$

If the problem is feasible, $\mathbf{J_{zz}} > 0$, and $\tilde{\mathbf{G}}^y$ invertible, we can find $\mathbf{c} = \mathbf{Hy}$ such that controlling $\mathbf{c}$ to zero yields optimal operation.

[1] V. Alstad, S. Skogestad and E. Hori., Optimal measurement combinations as controlled variables. *J. Proc. Contr., 2008*

Proof I

- First order optimality conditions (KKT-conditions):

$$[\mathbf{A}_z\,,\mathbf{A}_d]\begin{bmatrix}\mathbf{z}\\ \mathbf{d}\end{bmatrix}-\mathbf{b}=0 \tag{1}$$

$$\nabla L=\mathbf{J_{zz}z}+\mathbf{J_{zd}d}+\mathbf{A}_z^{\mathbf{T}}\lambda$$
$$\nabla L=\tilde{J}\begin{bmatrix}\mathbf{z}\\ \mathbf{d}\end{bmatrix}+\mathbf{A}_z^{\mathbf{T}}\lambda=0 \tag{2}$$

- $\mathbf{A}_z\in\mathbb{R}^{n_c\times n_z}$, $\lambda\in\mathbb{R}^{n_c\times 1}$, and $n_c<n_z$, equation (2) is linear and overdetermined in λ.

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- $\mathbf{A}_z\in\mathbb{R}^{n_c\times n_z}$, $\lambda\in\mathbb{R}^{n_c\times 1}$, and $n_c<n_z$, equation (2) is linear and overdetermined in λ.
- To be able solve for λ, we must have at the optimum:

$$\mathbf{c}_s^v=\mathbf{N}_z^{\mathbf{T}}\tilde{J}\begin{bmatrix}\mathbf{z}\\ \mathbf{d}\end{bmatrix}=0 \tag{3}$$

- $\mathbf{N}_z$ basis for the null space of constraint Jacobian $\mathbf{A}_z$

Proof II

- At optimal operation the invariant variable combination is

$$\mathbf{c}_s^v = \mathbf{N}_z^{\mathbf{T}} \tilde{J} \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix} = 0$$

Proof II

- At optimal operation the invariant variable combination is

$$\mathbf{c}_s^v = \mathbf{N}_z^{\mathbf{T}} \tilde{J} \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix} = 0$$

- Using the measurements: $\mathbf{y} = \tilde{\mathbf{G}}^y \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix}$ we get the

  invariant measurement combination:

$$\begin{aligned} \mathbf{c}_s^y &= \mathbf{N}_z^{\mathbf{T}} \tilde{J} [\tilde{\mathbf{G}}^y]^{-1} \mathbf{y} \\ \mathbf{c}_s^y &= \mathbf{H}\mathbf{y} \end{aligned} \quad (4)$$

□

Modified Null-Space Method – Nonlinear case

Theorem

Given a nonlinear optimization problem

$$\min_{\mathbf{z}} J(\mathbf{z}, \mathbf{d})$$

$$s.t$$

$$a_{c,i}(\mathbf{z}, \mathbf{d}) = 0, \quad i = 1 \dots n_c$$

with implicit measurements

$$p_{y,j}(\mathbf{y}, \mathbf{z}, \mathbf{d}) = 0.$$

If the Jacobian of the constraints $\mathbf{A}^{\mathbf{T}} = \left[\nabla p_{c,i}\right]$ *has constant rank* n_c*, there are* $n_{DOF} = n_z - n_c$ *independent invariant variable combinations* c_s^v*.*

Modified Null-space Method – Nonlinear case

Proof.

- $\nabla_z L = \nabla_z J + \mathbf{A}_z^{\mathbf{T}} \lambda$ $\qquad \mathbf{A}_z = \begin{bmatrix} \nabla_z p_{c,1}(\mathbf{z}, \mathbf{d}) \\ \vdots \\ \nabla_z p_{c,n_c}(\mathbf{z}, \mathbf{d}) \end{bmatrix}$
- For existence and uniqueness of λ we must have:

$$[\mathbf{N}_z(\mathbf{z}, \mathbf{d})]^{\mathbf{T}} \nabla_z J(\mathbf{z}, \mathbf{d}) = [\mathbf{A}_z(\mathbf{z}, \mathbf{d})]^{\mathbf{T}} \lambda = 0 \qquad (5)$$

- $\mathbf{N}_z(\mathbf{z}, \mathbf{d})$ chosen as a basis for the null space of $\mathbf{A}_z(\mathbf{z}, \mathbf{d})$
- Invariant variable combinations:

$$c_s^v = [\mathbf{N}(\mathbf{z}, \mathbf{d})]^{\mathbf{T}} \nabla_z J(\mathbf{z}, \mathbf{d}) = 0$$

- If unknowns can be eliminated, invariant is used for control

□

Eliminating unknowns – polynomial case

- System equations:

$$\begin{aligned} \mathbf{N}^T \nabla J(\mathbf{u}, \mathbf{x}, \mathbf{d}) &= 0 \\ p_{c,i}(\mathbf{u}, \mathbf{x}, \mathbf{d}) &= 0 \\ p_{y,j}(\mathbf{y}, \mathbf{u}, \mathbf{x}, \mathbf{d}) &= 0 \end{aligned}$$

- Eliminating the unknowns:
  $c_s^v = [\mathbf{N}^T \nabla J(\mathbf{u}, \mathbf{x}, \mathbf{d})]_k = \sum_{i,j} h_{c,i} \underbrace{p_{c,i}} + g_{y,j} \underbrace{p_{y,j}} + r_k(\mathbf{y})$

- Existence of $h_{c,k}$ and $g_{y,k}$ is determined using Gröbner bases and polynomial division.

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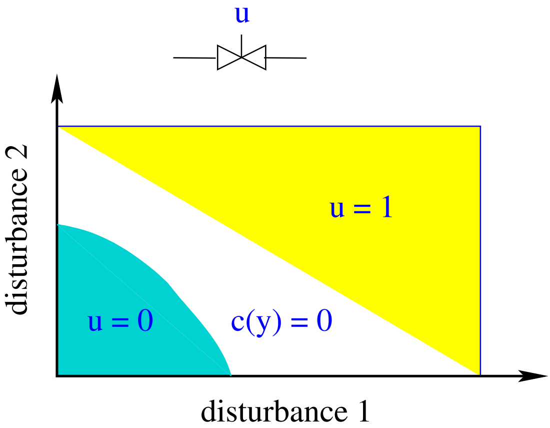
Changing sets of active constraints

- Usually several sets of active constrains
- How to know when to change the active set?



Changing Regions

Theorem (Changing Regions)

Assume the system is operated optimally and the disturbance moves the system gradually over the region boundary (no region can be jumped over), the switching instants and the new regions can be detected by monitoring

- *the active constraints, and*
- *the invariant variable combinations*

of the neighbouring regions.

Proof I

- Define two types of transitions from region 1 to region 2:
  - Type I: An active constraint is added or replaced

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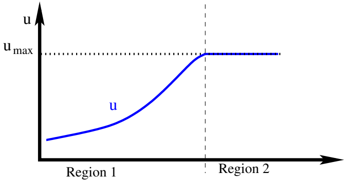
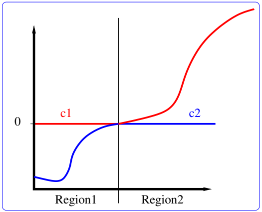
- Type I: Change when constraint is hit



Proof II

Type II: Change when invariant reaches zero and keep it at zero



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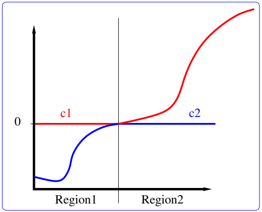


Show $c_{s,2} \neq 0$ inside region 1:

- Assume system in region 1, $c_{s,1} = 0$ and at $\mathbf{z}_0, \mathbf{d}_0$ $c_{s,2} = 0$.
- $[\mathbf{N}_1(\mathbf{z}_0, \mathbf{d}_0)]^{\mathbf{T}} \nabla_z J(\mathbf{z}_0, \mathbf{d}_0) = [\mathbf{N}_2(\mathbf{z}_0, \mathbf{d}_0)]^{\mathbf{T}} \nabla_z J(\mathbf{z}_0, \mathbf{d}_0)$
- Null spaces of $\mathbf{A}_1(\mathbf{z}_0, \mathbf{d}_0)$ and $\mathbf{A}_2(\mathbf{z}_0, \mathbf{d}_0)$ have same basis
- $\mathbf{A}_1(\mathbf{z}_0, \mathbf{d}_0)$ and $\mathbf{A}_2(\mathbf{z}_0, \mathbf{d}_0)$ are row equivalent
- Impossible, because the constant rank condition on $\mathbf{A}_1$ and $\mathbf{A}_2$, and fewer active constraints give $\mathrm{rank}(\mathbf{A}_2) < \mathrm{rank}(\mathbf{A}_1)$.

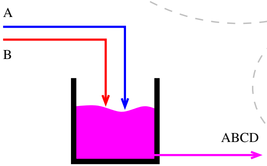
CSTR Example [2]

Two reactions:
$$\begin{aligned} A + B &\xrightarrow{k_1} C \\ 2\,B &\xrightarrow{k_2} D \end{aligned}$$

$$\max_{F_A, F_B} \frac{(F_A + F_B)c_c}{F_A c_{A_{in}}}(F_A + F_B)c_c$$

s.t.

$$\begin{aligned} F_A c_{A_{in}} - (F_A + F_B)c_A - k_1 c_A c_B V &= 0 \\ F_B c_{B_{in}} - (F_A + F_B)c_B - k_1 c_A c_B V - 2k_2 c_B^2 V &= 0 \\ -(F_A + F_B)c_C + k_1 c_A c_B V &= 0 \\ F_A + F_B - F &= 0 \\ k_1 c_A c_B V(-\Delta H_1) + 2k_2 c_B V(-\Delta H_2) - q &= 0 \\ q - q_{\max} &\leq 0 \\ F - F_{\max} &\leq 0 \end{aligned}$$

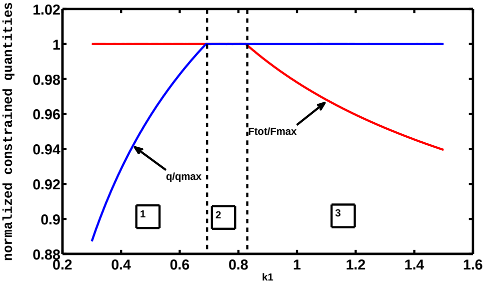


- Manipulated **u**: F_A, F_B
- Measured **y**: F_A, F_B, c_B, q
- Unknown **d**: rate constant k_1

[2] B. Srinivasan, L.T. Biegler, and D. Bonvin. Tracking the necessary conditions of optimality with changing set of active constraints using a barrier-penalty function. *Computers and Chemical Engineering, 2008*

CSTR Example I

2 DOF, three regions of active constraints:



Disturbance	Region	Active constraints	#unconstr DOF
$k_1 < 0.65$	Region 1	$F = F_{max}$	1 ($c^y_{s,1}$)
$0.65 \leq k_1 \leq 0.8$	Region 2	$F = F_{max}$, $q = q_{max}$	0 (–)
$0.8 < k_1$	Region 3	$q = q_{max}$	1 ($c^y_{s,3}$)

CSTR Example II

Region 1

$$
\begin{aligned}
F &= F_{max} \\
c_{s,1} &= -F_{max}(F_{max}c_B + 2c_B^2k_2V - F_Bc_{B,in})^2 \\
&\quad (4c_B^4k_2^2V^2 + 4F_{max}c_B^3k_2V - 6k_2Vc_B^2F_Bc_{A,in} \\
&\quad - 4k_2VF_{max}c_{B,in}c_B^2 + 6k_2Vc_B^2F_{max}c_{A,in} \\
&\quad + F_{max}^2c_B^2 - 2F_{max}^2c_{B,in}c_B + 2c_BF_{max}^2c_{A,in} \\
&\quad - 2c_BF_{max}F_Bc_{A,in} - F_B^2c_{B,in}^2 + 3F_{max}F_Bc_{A,in}c_{B,in} \\
&\quad - F_B^2c_{A,in}c_{B,in} + 2F_{max}F_Bc_{B,in}^2 - 2F_{max}^2c_{A,in}c_{B,in})
\end{aligned}
$$

Region 3

$$
\begin{aligned}
q &= q_{max} \\
c_{s,3} &= -(F_Ac_B + c_BF_B + 2c_B^2k_2V - c_{B,in}F_B)^2 \\
&\quad (-3F_B^2q_{max}c_{B,in}c_B + 8c_B^4q_{max}k_2^2V^2 \\
&\quad + F_B^2q_{max}c_{B,in}^2 + 2c_B^2F_B^2q_{max} + 2F_A^2q_{max}c_B^2 \\
&\quad + 4c_B^4F_Bk_2^2c_{B,in}V^2\Delta H_2 + 8c_B^3F_Bq_{max}k_2V \\
&\quad + 2c_B^3F_B^2k_2c_{B,in}V\Delta H_2 - 6c_B^2F_Bq_{max}k_2c_{B,in}V \\
&\quad - 2c_B^2F_B^2k_2c_{B,in}^2V\Delta H_2 - F_A^2q_{max}c_{B,in}c_B \\
&\quad + 4F_Ac_B^2F_Bq_{max} + F_AF_Bq_{max}c_{B,in}^2 + 2F_A^2c_Bq_{max}c_{A,in} \\
&\quad + 6F_A^2k_2c_{B,in}V\Delta H_2c_B^3 + 12F_Ak_2^2c_{B,in}V^2\Delta H_2c_B^4 \\
&\quad + 8F_Ac_B^3F_Bk_2c_{B,in}V\Delta H_2 + 8F_Ac_B^3q_{max}k_2V \\
&\quad - 2F_Ac_B^2q_{max}k_2c_{B,in}V - 6F_Ac_B^2F_Bk_2c_{B,in}^2V\Delta H_2 \\
&\quad - 4F_AF_Bq_{max}c_{B,in}c_B + 2F_A^2c_B^2k_2c_{A,in}c_{B,in}V\Delta H_2 \\
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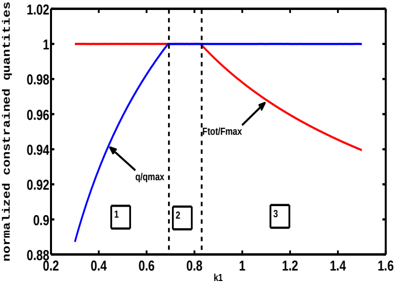
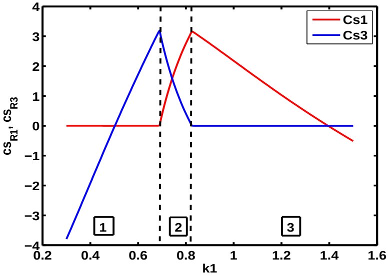
&\quad + 4F_Ac_B^3F_Bk_2c_{A,in}V\Delta H_2 - 2F_Ac_B^2F_Bk_2c_{A,in}c_{B,in}V\Delta H_2 \\
&\quad + 4F_Ac_B^2q_{max}k_2c_{A,in}V + 2F_Ac_BF_Bq_{max}c_{A,in}
\end{aligned}
$$

CSTR Example III

Changing regions

	Region 1	Region 2	Region 3
DOF 1	$F/F_{max} = 1$	$F/F_{max} = 1$	$c^y_{s,3} = 0$
DOF 2	$c^y_{s,1} = 0$	$q/q_{max} = 1$	$q/q_{max} = 1$





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- Optimally invariant variable combinations can be found for non-linear systems
- If the measurements give information about internal states and the disturbances we can obtain measurement invariants
- It is possible to track regions by tracking the controlled variables of the neighbouring region.

Thank you for your attention