# Explicit Real-Time Optimization

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Innovation and Creativity

# Outline

- Introduction
  - Optimizing Control Concepts
- Motivating Example
- Null-Space method - constrained
- Nonlinear extension
- CSTR-Example

# Real-Time Optimization

- Process control strategy to optimize process performance
- Nonlinear steady state models
- Optimizes (nonlinear) process model performance on-line, in real-time
- Computed optimal setpoints are implemented in the process

# Optimizing Control Concepts

## On-line Optimization - Conventional RTO

- Optimal operation is achieved by using measurements to update a process model at given sample times
- The model is optimized on-line, and the computed inputs are implemented

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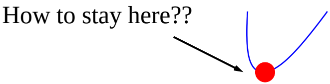
## Off-line Optimization - Explicit RTO




- Precomputed solutions are used
- For each set of active constraints we find invariant variable combinations, which yield optimal operation at their set-points
- These variables can be be controlled by simple PID controllers
- No need for expensive real-time computations

## 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 $\mathbf{c}_s^y = f(\mathbf{y})$

## Motivating example

- $\min f(u,d) = \min u_1(u_1 - 2d_2) + u_2(u_2 - d_1)$
- With measurements:

$$y_1 = \frac{2}{u_1 d_1}(d_2 - d_1^2 - 1) \longrightarrow p_1^y = \frac{1}{2} y_1 u_1 d_1 - d_2 + d_1^2 + 1$$

$$y_2 = \frac{1}{u_1}(d_1 - 1) \longrightarrow p_2^y = y_2 u_1 - d_1 + 1$$

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Invariant variable combinations:

- $c_1^v = 2(u_1 - d_2) = 0$
- $c_2^v = 2(u_2 - d_1) = 0$

## Motivating example

- $G_y$ for $<_{lex}$ with $d_1 > d_2 > u_1 > u2 > y_1 > y2$:

$$
\begin{aligned}
g_1 &= 2d_2 - u_1^2 y_1 y_2 + 2u_1^2 y_2^2 - u_1 y_1 + 4u_1 y_2 \\
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- 1. Measurement invariant: divide $c_1^y$ by $G^y = \{g_1, g_2\} \longrightarrow c_{s,1}^y$
- 2. Measurement invariant: divide $c_2^y$ by $G^y = \{g_1, g_2\} \longrightarrow c_{s,2}^y$

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Invariant measurement combinations:

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

# Null-space method (extension of [1])

## Theorem (Quadratic objective, linear constraints)

*Consider the optimization problem:*

$$\min \, [\mathbf{u}^{\mathrm{T}}\mathbf{x}^{\mathrm{T}}\mathbf{d}^{\mathrm{T}}] \underbrace{\begin{bmatrix} & \mathbf{DJ} & \\ \mathbf{J_{ud}}^{\mathrm{T}} & \mathbf{J_{xd}}^{\mathrm{T}} & \mathbf{J_{dd}} \end{bmatrix}}_{\mathbf{Q}} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \\ \mathbf{d} \end{bmatrix}$$

$$\textit{s.t.} \quad [\mathbf{A}\,,\mathbf{A}_d] \begin{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \end{bmatrix} \\ \mathbf{d} \end{bmatrix} = \mathbf{b} \textit{ with measurements}$$

$$\mathbf{y} = \mathbf{G}^y\mathbf{u} + \mathbf{G}^y_x\mathbf{x} + \mathbf{G}^y_d\mathbf{d} = \tilde{\mathbf{G}}^y \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \\ \mathbf{d} \end{bmatrix}$$

*If the problem is feasible,* $\mathbf{Q} > 0$*, 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. *Journal of Process Control, 2008*

## Proof I

- First order optimality conditions:

$$
\begin{aligned}
0 &= [\mathbf{A}\,, \mathbf{A}_d]\,[\mathbf{u}\,\mathbf{x}\,\mathbf{d}]^{\mathrm{T}} - \mathbf{b} \\
\nabla L &= \mathbf{A}^{\mathrm{T}}\lambda + \mathbf{DJ}\begin{bmatrix}\mathbf{u}\\ \mathbf{x}\\ \mathbf{d}\end{bmatrix} = 0
\end{aligned}
\tag{1}
$$

- $\mathbf{A} \in \mathbb{R}^{n_c \times n_u + n_x}$, Degrees of freedom $n_{DOF} = n_u + n_x - n_c > 0$

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- Row-reduce second equation such that $\mathbf{EA}^{\mathrm{T}} = \mathbf{R}$:

$$
\mathbf{E}\nabla L = \underbrace{\mathbf{EA}^{\mathrm{T}}}_{\mathbf{R}}\lambda + \mathbf{EDJ}\begin{bmatrix}\mathbf{u}\\ \mathbf{x}\\ \mathbf{d}\end{bmatrix} = 0 \tag{2}
$$

- $\mathbf{R}$ upper triangular and last $n_{DOF}$ rows are zero

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- $\mathbf{R}$ upper triangular and last $n_{DOF}$ rows are zero
- Last $n_{DOF}$ rows in $\mathbf{E}$ are basis for left null space of $\mathbf{A}^{\mathrm{T}}$, and the null space of $\mathbf{A}$

## Proof II

- Select **N** in the null space of **A**, the last $n_{DOF}$ rows of $\nabla L = 0$ become:

$$\mathbf{N}^\mathbf{T}\nabla L = \underbrace{\mathbf{N}^\mathbf{T}\mathbf{A}^\mathrm{T}}_{=0}\lambda + \mathbf{N}^\mathbf{T}\mathbf{D}\mathbf{J}\begin{bmatrix}\mathbf{u}\\ \mathbf{x}\\ \mathbf{d}\end{bmatrix}$$

- At optimal operation we have the invariant variable combination $c_s^v$

$$c_s^v = \mathbf{N}^\mathbf{T}\mathbf{D}\mathbf{J}\begin{bmatrix}\mathbf{u}\\ \mathbf{x}\\ \mathbf{d}\end{bmatrix} = 0$$

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- Using $\mathbf{y} = \tilde{\mathbf{G}}^y\begin{bmatrix}\mathbf{u}\\ \mathbf{x}\\ \mathbf{d}\end{bmatrix}$ with $\tilde{\mathbf{G}}^y$ invertible we have the invariant measurement combination $c_s^y$

$$c_s^y = \mathbf{N}^{\mathbf{T}}\mathbf{DJ}[\tilde{\mathbf{G}}^y]^{-1}\mathbf{y} = \mathbf{H}\mathbf{y}$$

## Nonlinear (Polynomial) case

**Theorem**

*Given a polynomial optimization problem*

$$\min f(\mathbf{u},\mathbf{x},\mathbf{d}) \quad \text{s.t} \quad p_{c,i}(\mathbf{u},\mathbf{x},\mathbf{d}) = 0 \quad i = 1 \dots n_c$$

*with implicit measurements* $p_{y,j}(\mathbf{y},\mathbf{u},\mathbf{x},\mathbf{d}) = 0$.
*If* $\mathbf{A}^\mathbf{T} = \left[\nabla p_{c,i}\right]$ *has constant rank* $n_c$ *there are* $n_{DOF} = n_u + n_x - n_c$ *independent invariant variable combinations* $c_s^v$.
*Furthermore if for every* $c_s^v$ *there exist some* $h_{c,i}, g_{y,j}$ *such it can be written in the form* $c_s^v = \sum_{i,j}\left(h_{c,i}p_{c,i} + g_{y,j}p_{y,j}\right) + r(\mathbf{y})$,
*the term* $r(\mathbf{y})$ *is the desired measurement invariant* $c_s^y$.

## Nonlinear case

### Proof part 1 - finding invariant variables $c_s^v$.

- $\nabla L = \nabla f + \mathbf{A}^\mathbf{T}\lambda \qquad \mathbf{A} = \begin{bmatrix} \nabla p_{c,1}(\mathbf{u},\mathbf{x},\mathbf{d}) \\ \vdots \\ \nabla p_{c,n_c}(\mathbf{u},\mathbf{x},\mathbf{d}) \end{bmatrix}$
- Row reduction: $\mathbf{EA}^\mathbf{T} = \mathbf{R}$, last $n_{DOF} = n_u + n_x - n_c$ rows of $\mathbf{E}$ form basis of left null-space of $\mathbf{A}^\mathbf{T}$
- Multiply: $\mathbf{N}^\mathbf{T}\nabla f(\mathbf{u},\mathbf{x},\mathbf{d}) + \underbrace{\mathbf{N}^\mathbf{T}\mathbf{A}^\mathbf{T}\lambda}_{=0}$
- $\mathbf{N}$ is basis for null space of $\mathbf{A}$
- Invariant variable combinations: $c_s^v = \mathbf{N}^\mathbf{T}\nabla f(\mathbf{u},\mathbf{x},\mathbf{d})$

$$\begin{aligned} c_s = \mathbf{N}^T\nabla f(\mathbf{u},\mathbf{x},\mathbf{d}) &= 0 \quad \#n_{DOF} \\ p_{c,i}(\mathbf{u},\mathbf{x},\mathbf{d}) &= 0 \quad \#n_c \end{aligned} \tag{3}$$

## Polynomial case

Proof part 2 - representing the invariants by measurements.

$$\mathbf{N}^T \nabla f(\mathbf{u}, \mathbf{x}, \mathbf{d}) = 0 \quad \# n_u + n_x - n_c$$
$$p_{c,i}(\mathbf{y}, \mathbf{u}, \mathbf{x}, \mathbf{d}) = 0 \quad \# n_c$$
$$p_{y,j}(\mathbf{y}, \mathbf{u}, \mathbf{x}, \mathbf{d}) = 0 \quad \# n_y$$

- $c_s^v = [\mathbf{N}^T \nabla f(\mathbf{u}, \mathbf{x}, \mathbf{d})]_k = \sum_{i,j} h_{c,i} \underbrace{p_{c,i}}_{=0} + g_{y,j} \underbrace{p_{y,j}}_{=0} + r_k(\mathbf{y})$
- Existence of $h_{c,k}$ and $g_{y,k}$ is determined using Gröbner bases and polynomial division. Given a term ordering ranking terms with **d** and **x** highest, all terms in $c_{s,k}$ with **x** and **d** can be formed by the initial term of some $\sum (\alpha p_{c,i} + \beta p_{y,j})$.

# CSTR Example [2]

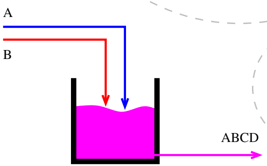
Two reactions:

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

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

s.t.

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



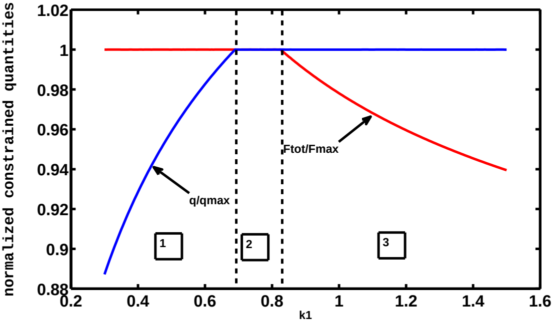

- Manipulated **u**: $F_A$, $F_B$
- Measured **y**: $F_A$, $F_B$, $c_A$, $q$
- Unknown **d**: rate constant $k_1$

[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

$F = F_{max}$

$c^y_{s,1} = 1.0204 - 0.36771F_B - 0.89003c_a + 3.43 \cdot 10^8 F_B^6 - 3.7961 \cdot 10^6 F_B^5 + 6.468 \cdot 10^7 F_B^5 c_a + 0.0001724F_B^4 - 0.11055c_a^2 - 5.082 \cdot 10^7 F_B^4 c_a^2 - 0.0041027F_B^3 + 0.22818c_a^3 - 5.9629 \cdot 10^5 F_B^3 c_a^3 + 0.053809F_B^2 + 0.00070862c_a^4 - 0.00015373F_B^2 c_a^4 - 0.029762c_a^5 + 0.0013528F_B c_a^5 + 0.0049604c_a^6 - 5.687 \cdot 10^5 F_B^4 c_a + 6.5086 \cdot 10^5 F_B^3 c_a^2 + 0.0030951F_B^2 c_a^3 + 0.0033499F_B c_a^4 + 0.0019587F_B^3 c_a - 0.0023543F_B^2 c_a^2 - 0.049604F_B c_a^3 - 0.032995F_B^2 c_a + 0.030729F_B c_a^2 + 0.27237F_B c_a$

## Region 3

$q = q_{max}$

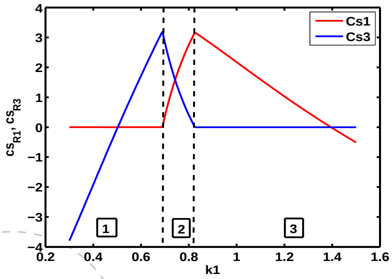
$c^y_{s,3} = 8c_a^4 F_B F^4 \Delta H_1^2 - 8c_a^4 F^5 \Delta H_1^2 - 14c_a^4 F_A F_B F^3 \Delta H_1 \Delta H_2 - 14c_a^4 F_B^2 F^3 \Delta H_1 \Delta H_2 + 17c_a^4 F_A F^4 \Delta H_1 \Delta H_2 + 17c_a^4 F_B F^4 \Delta H_1 \Delta H_2 + 48c_a^3 F_A F_B^2 F^2 \Delta H_1^2 + 48c_a^3 F_B^3 F^2 \Delta H_1^2 - 112c_a^3 F_A F_B F^3 \Delta H_1^2 - 96c_a^3 F_B^2 F^3 \Delta H_1^2 + 64c_a^3 F_A F^4 \Delta H_1^2 + 48c_a^3 F_B F^4 \Delta H_1^2 - 72c_a^3 F_A F_B^2 F^2 \Delta H_1 \Delta H_2 - 72c_a^3 F_B^3 F^2 \Delta H_1 \Delta H_2 + 196c_a^3 F_A F_B F^3 \Delta H_1 \Delta H_2 + 156c_a^3 F_B^2 F^3 \Delta H_1 \Delta H_2 - 130c_a^3 F_A F^4 \Delta H_1 \Delta H_2 - 84c_a^3 F_B F^4 \Delta H_1 \Delta H_2 + 6c_a^3 F_A F_B^2 F^2 \Delta H_2^2 + 6c_a^3 F_B^3 F^2 \Delta H_2^2 - 6c_a^3 F_A F_B F^3 \Delta H_2^2 - 12c_a^3 F_B^2 F^3 \Delta H_2^2 + 6c_a^3 F_B F^4 \Delta H_2^2 + 4c_a^4 F_A F^3 \Delta H_2 q_{max} + 4c_a^4 F_B F^3 \Delta H_2 q_{max} + 96c_a^2 F_A F_B^3 F \Delta H_1^2 + 96c_a^2 F_B^4 F \Delta H_1^2 - 384c_a^2 F_A F_B^2 F^2 \Delta H_1^2 - 288c_a^2 F_B^3 F^2 \Delta H_1^2 + 480c_a^2 F_A F_B F^3 \Delta H_1^2 + 288c_a^2 F_B^2 F^3 \Delta H_1^2 - 192c_a^2 F_A F^4 \Delta H_1^2 - 96c_a^2 F_B F^4 \Delta H_1^2 - 120c_a^2 F_A F_B^3 F \Delta H_1 \Delta H_2 \ldots$

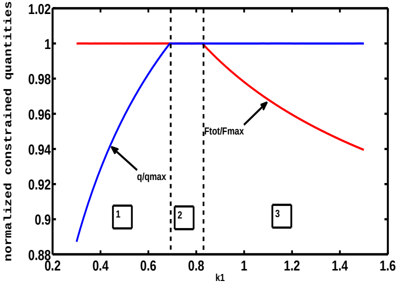
- Region 2:
  $F = F_{max}$, $q = q_{max}$
- only known variables and parameters in the invariants

# CSTR Example III

## How do we know when to change 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
- For the CSTR example it is possible to track regions by tracking the controlled variables of the neighbouring region

Thank you for your attention