Explicit Real-Time Optimization

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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
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

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 controlled by simple PID controllers
- No need for expensive real-time computations

How to stay here??
Explicit RTO procedure

1. Formulate the optimization problem:
   \[
   \min f(u, x, d) \text{ s.t. } g(u, x, d) \leq 0 \text{ and } h(u, x, d) = 0
   \]

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 \( c_s^y = f(y) \)
Motivating example

- \( \min f(u, d) = \min u_1(u_1 - 2d_2) + u_2(u_2 - d_1) \)
- With measurements:
  \[
  \begin{align*}
  y_1 &= \frac{2}{u_1 d_1} (d_2 - d_1^2 - 1) \\
  y_2 &= \frac{1}{u_1} (d_1 - 1)
  \end{align*}
  \]
  \[
  \begin{align*}
  p_1^y &= \frac{1}{2} y_1 u_1 d_1 - d_2 + d_1^2 + 1 \\
  p_2^y &= y_2 u_1 - d_1 + 1
  \end{align*}
  \]
Motivating example

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- With measurements:
  \[
  y_1 = \frac{2}{u_1d_1}(d_2 - d_1^2 - 1) \quad \rightarrow \quad p_1^y = \frac{1}{2} y_1 u_1 d_1 - d_2 + d_1^2 + 1 \\
  y_2 = \frac{1}{u_1}(d_1 - 1) \quad \rightarrow \quad p_2^y = y_2 u_1 - d_1 + 1
  \]

Invariant variable combinations:

- \( c_1^y = 2(u_1 - d_2) = 0 \)
- \( c_2^y = 2(u_2 - d_1) = 0 \)
Motivating example

- $G_y$ for $<_\text{lex}$ with $d_1 > d_2 > u_1 > u_2 > y_1 > y_2$:
  
  \[
  g_1 = 2d_2 - u_1^2 y_1 y_2 + 2u_1^2 y_2^2 - u_1 y_1 + 4u_1 y_2 \\
  g_2 = d_1 - u_1 y_2 - 1
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  \]

- 1. Measurement invariant: divide $c_1^y$ by $G^y = \{g_1, g_2\} \rightarrow c_{s,1}^y$
- 2. Measurement invariant: divide $c_2^y$ by $G^y = \{g_1, g_2\} \rightarrow c_{s,2}^y$
Motivating example

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- 1. Measurement invariant: divide $c_1^y$ by $G^y = \{g_1, g_2\} \rightarrow c_{s,1}^y$
- 2. Measurement invariant: divide $c_2^y$ by $G^y = \{g_1, g_2\} \rightarrow c_{s,2}^y$

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:

\[
\min \left[ u^T x^T d^T \right]
\begin{bmatrix}
\underbrace{J_{ud}^T & DJ & J_{xd}^T & J_{dd}}_Q
\end{bmatrix}
\begin{bmatrix}
u \\
x \\
d
\end{bmatrix}
\]

s.t. \quad \begin{bmatrix}
u \\
x \\
d
\end{bmatrix}
\begin{bmatrix}
A \\
A_d
\end{bmatrix}
= b \quad with \ measurements

\[
y = G^y u + G_x^y x + G_d^y d = \tilde{G}^y
\begin{bmatrix}
u \\
x \\
d
\end{bmatrix}
\]

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

Proof I

- First order optimality conditions:

\[ 0 = \left[ A, A_d \right] \left[ u \times d \right]^T - b \]

\[ \nabla L = A^T \lambda + DJ \begin{bmatrix} u \\ x \\ d \end{bmatrix} = 0 \] (1)

- \( A \in \mathbb{R}^{n_c \times n_u + n_x} \), Degrees of freedom \( n_{DOF} = n_u + n_x - n_c > 0 \)
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- Row-reduce second equation such that \( EA^T = R \):

\[
E \nabla L = \underbrace{EA^T}_{R} \lambda + EDJ \begin{bmatrix} u \\ x \\ d \end{bmatrix} = 0
\] (2)

- \( R \) upper triangular and last \( n_{DOF} \) rows are zero
Proof I

- First order optimality conditions:
  \[ 0 = [A, A_d] [u \times d]^T - b \]
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  \]

- \( R \) upper triangular and last \( n_{DOF} \) rows are zero

- Last \( n_{DOF} \) rows in \( E \) are basis for left null space of \( A^T \), and the null space of \( A \)
Proof II

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

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

- At optimal operation we have the invariant variable combination $c^V_s$

$$c^V_s = \mathbf{N}^T \mathbf{D} \mathbf{J} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \\ \mathbf{d} \end{bmatrix} = 0$$
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\]

• At optimal operation we have the invariant variable combination $c_v^s$

\[
c_v^s = \mathbf{N}^T \mathbf{D} \mathbf{J} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \\ \mathbf{d} \end{bmatrix} = 0
\]

• 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 $c_s^y$

\[
c_s^y = \mathbf{N}^T \mathbf{D} \mathbf{J} [\tilde{\mathbf{G}}^y]^{-1} \mathbf{y} = \mathbf{H} \mathbf{y}
\]
Nonlinear (Polynomial) case

Theorem

Given a polynomial optimization problem

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

with implicit measurements $$p_{y,j}(y, u, x, d) = 0$$. If $$A^T = [\nabla p_{c,i}]$$ 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 $$c_s^v = \sum_{i,j} (h_{c,i}p_{c,i} + g_{y,j}p_{y,j}) + r(y)$$, the term $$r(y)$$ is the desired measurement invariant $$c_s^v$$. 
Nonlinear case

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

- $\nabla L = \nabla f + A^T \lambda$
  
  $A = \begin{bmatrix}
  \nabla p_{c,1}(u, x, d) \\
  \vdots \\
  \nabla p_{c,n_c}(u, x, d)
  \end{bmatrix}$

- Row reduction: $EA^T = R$, last $n_{DOF} = n_u + n_x - n_c$ rows of $E$ form basis of left null-space of $A^T$

- Multiply: $N^T \nabla f(u, x, d) + N^T A^T \lambda = 0$
  
  $N$ is basis for null space of $A$

- Invariant variable combinations: $c_s^v = N^T \nabla f(u, x, d)$

\[ c_s = N^T \nabla f(u, x, d) = 0 \quad \# n_{DOF} \]
\[ p_{c,i}(u, x, d) = 0 \quad \# n_c \]
Polynomial case

Proof part 2 - representing the invariants by measurements.

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

- \( c_s^y = [N^T \nabla f(u, x, d)]_k = \sum_{i,j} h_{c,i} p_{c,i} + g_{y,j} p_{y,j} + r_k(y) \)
  \[ = 0 \]
  \[ = 0 \]

- 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:

\[ \begin{align*}
\text{A} + \text{B} & \xrightarrow{k_1} \text{C} \\
2 \text{B} & \xrightarrow{k_2} \text{D}
\end{align*} \]

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

s.t.

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

## CSTR Example I

2 DOF, three regions of active constraints:

<table>
<thead>
<tr>
<th>Disturbance</th>
<th>Region</th>
<th>Active constraints</th>
<th>#unconstr DOF</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_1 &lt; 0.65$</td>
<td>Region 1</td>
<td>$F = F_{\text{max}}$</td>
<td>$1$ ($c_{s,1}^y$)</td>
</tr>
<tr>
<td>$0.65 \leq k_1 \leq 0.8$</td>
<td>Region 2</td>
<td>$F = F_{\text{max}}$, $q = q_{\text{max}}$</td>
<td>$0$ (–)</td>
</tr>
<tr>
<td>$0.8 &lt; k_1$</td>
<td>Region 3</td>
<td>$q = q_{\text{max}}$</td>
<td>$1$ ($c_{s,3}^y$)</td>
</tr>
</tbody>
</table>

![Diagram showing normalized constrained quantities](chart.png)
CSTR Example II

Region 1

\[ F = F_{\text{max}} \]

\[ c_{s,1}^y = 1.0204 - 0.36771 F_B - 0.89003 c_a + 3.43 \cdot 10^8 F_B^6 - 3.7961 \cdot 10^6 F_B^5 + 6.468 \cdot 10^7 F_B^5 c_a + 0.0001724 F_B^4 - 0.11055 c_a^2 - 5.082 \cdot 10^7 c_a^2 + 0.0041027 F_B^3 + 0.22818 c_a^3 - 5.9629 \cdot 10^5 F_B c_a^3 + 0.053809 F_B^2 + 0.00070862 c_a^4 - 0.00015373 F_B^2 c_a^4 - 0.029762 c_a^5 + 0.0013528 F_B c_a^5 + 0.0049624 c_a^6 - 5.687 \cdot 10^5 F_B c_a + 6.5086 \cdot 10^5 F_B^2 c_a^2 + 0.0030951 F_B^2 c_a^3 + 0.0033499 F_B c_a^4 + 0.0019587 F_B^3 c_a - 0.0023543 F_B^2 c_a^2 - 0.049604 F_B c_a^3 - 0.032995 F_B^2 c_a + 0.030729 F_B c_a^2 + 0.27237 F_B c_a \]

- Region 2:

\[ F = F_{\text{max}}, \quad q = q_{\text{max}} \]

- only known variables and parameters in the invariants

Region 3

\[ q = q_{\text{max}} \]

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

How do we know when to change regions

<table>
<thead>
<tr>
<th>DOF 1</th>
<th>Region 1</th>
<th>Region 2</th>
<th>Region 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( F / F_{\text{max}} ) = 1</td>
<td>( F / F_{\text{max}} ) = 1</td>
<td>( c_{s,3}^y ) = 0</td>
<td></td>
</tr>
<tr>
<td>( c_{s,1}^y ) = 0</td>
<td>( q / q_{\text{max}} ) = 1</td>
<td>( q / q_{\text{max}} ) = 1</td>
<td></td>
</tr>
</tbody>
</table>

Diagram showing normalized constrained quantities for different regions.
Conclusion

- An explicit approach to Real Time Optimization has been presented
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- If the measurements give information about internal states and the disturbances we can obtain measurement invariants.
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• An explicit approach to Real Time Optimization has been presented

• 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