## **Self-optimizing control Theory**

«How to put optimization into the control layer by selecting the right controlled variable c»

Sigurd Skogestad 2025

### **Outline**

Skogestad procedure for control structure design:

#### I. Top Down

- Step S1: Define operational objective (cost) and constraints
- Step S2: Identify degrees of freedom and optimize operation for disturbances
- Step S3: Implementation of optimal operation
  - Control active constraints
  - Control self-optimizing variables for unconstrained, c=Hy
- Step S4: Where set the production rate? (Inventory control)

#### II. Bottom Up

- Step S5: Regulatory control: What more to control (secondary CV's)?
- <u>Step S6</u>: Supervisory control
- Step S7: Real-time optimization

### **Step S3**: Implementation of optimal operation

Optimal operation for given d\*:

$$\min_{u} J(u, x, d) \\
\longrightarrow u_{ont}$$

subject to:

Model equations: f(u, x, d) = 0

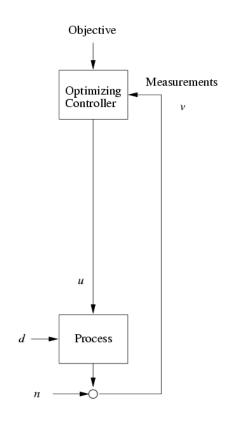
Operational constraints: g(u, x, d) < 0

*Problem:* Usally cannot keep  $u_{opt}$  constant because disturbances d change

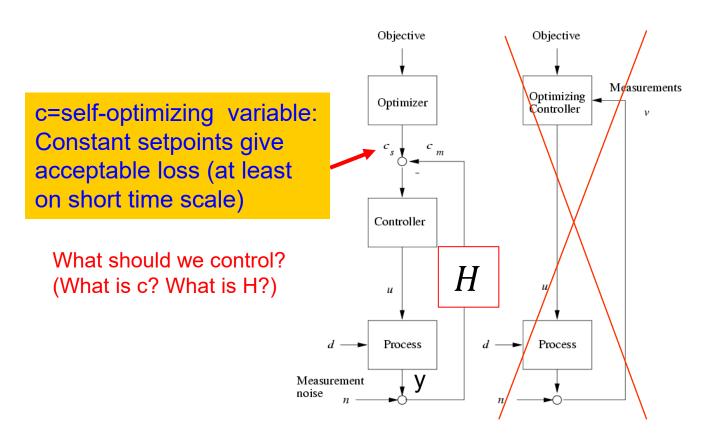
How should we adjust the degrees of freedom (u)?

What should we control?

# "Optimizing Control" (EMPC)



# "Self-Optimizing Control"



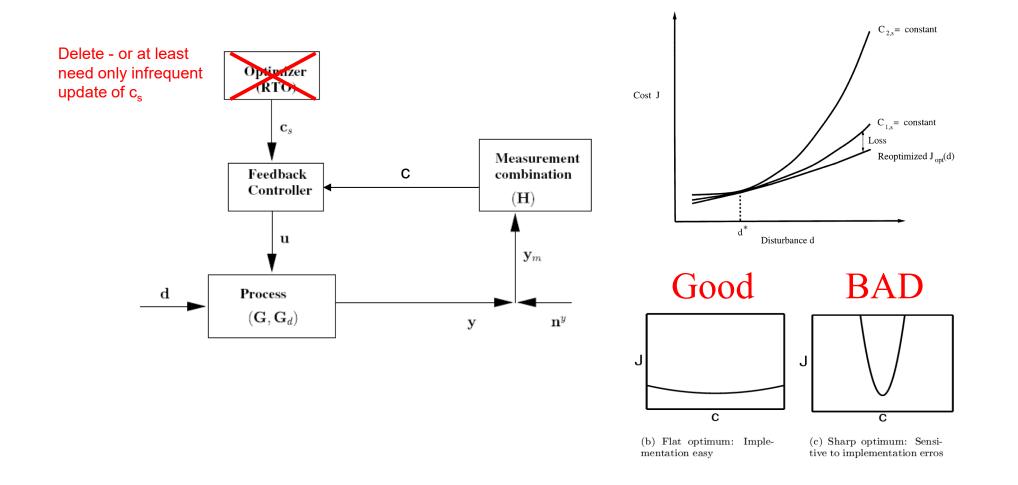
c = Hy

#### *H*: Nonsquare matrix

- Usually prefer single measurements as c's (simple)— H is selection matrix of 0's and 1's
- H can also be full matrix (measurement combinations)

## **Self-optimizing control**

Self-optimizing control is when we can achieve an acceptable loss with constant setpoint values for the controlled variables



# Optimal operation of runner

- Cost to be minimized: J = T (total time)
- One degree of freedom: u = power
- What should we control?



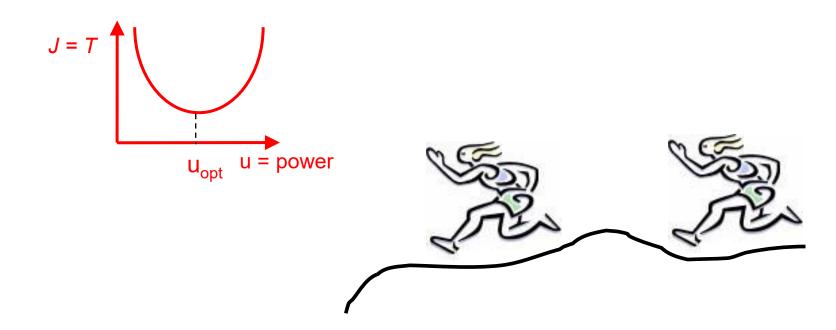
## 1. Sprinter case

- 100 meters run. J = T
- Active constraint control:
  - Maximum speed ("no thinking required")
  - CV = power (at max)



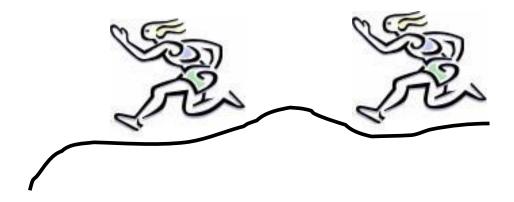
### 2. Marathon runner case

- 40 km run. J = T (total time)
- What should we control? CV = ?
- Unconstrained optimum:

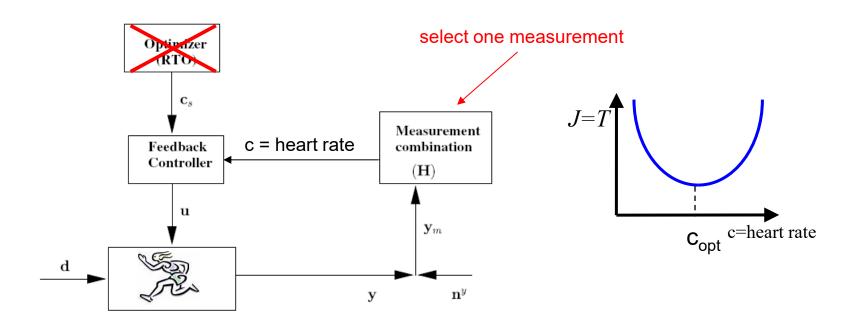


# Self-optimizing control: Marathon

- Any self-optimizing variable (to control at constant setpoint)?
  - $-c_1 = distance to leader of race (not optimal and not always feasible)$
  - $c_2$  = speed (not always feasible, similar to controlling cost J=T, speed = 42 km/T)
  - $-c_3$  = heart rate
  - $c_4 =$  «pain» = level of lactate in muscles



### **Conclusion Marathon runner**

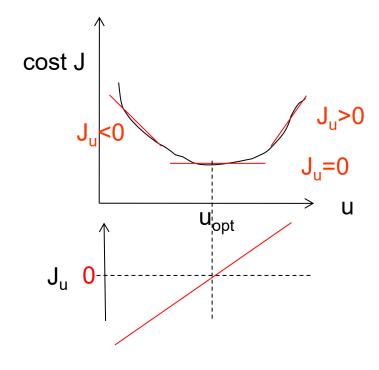


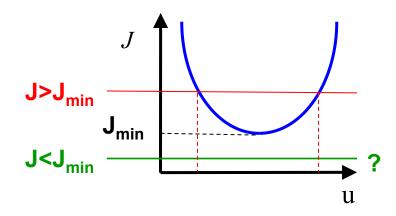
- CV = heart rate is good "self-optimizing" variable
- Simple and robust implementation
- Disturbances are indirectly handled by keeping a constant heart rate
- May have infrequent adjustment of setpoint (c<sub>s</sub>)

# The ideal "self-optimizing" variable is the gradient, $J_u$

$$c = \Delta J/\Delta u = Ju$$

- Keep gradient at zero for all disturbances ( $c = J_{\parallel} = 0$ )
- Problem: Usually no measurement of gradient





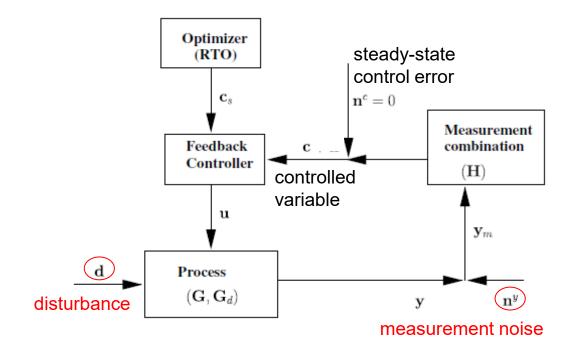
# Unconstrained optimum: **NEVER** try to control a variable that reaches max or min at the optimum

- In particular, never try to control directly the cost J
- Assume we want to minimize J (e.g., J = V = energy) and we make the stupid choice os selecting CV = V = J
  - Then setting J < J<sub>min</sub>: Gives infeasible operation (cannot meet constraints)
  - and setting  $J > J_{min}$ : Forces us to be nonoptimal (two steady states: may require strange operation)

#### Measurements or mesurement combinations

Ideally:  $c = J_u$ 

In practice: c = Hy



• Single measurements:

$$\mathbf{c} = \mathbf{H}\mathbf{y} \qquad \mathbf{H} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

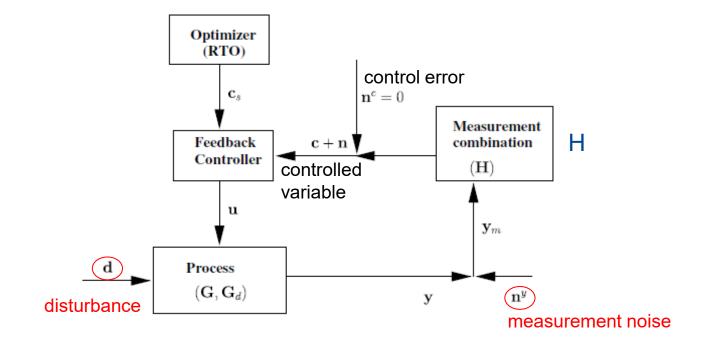
Combinations of measurements:

$$\mathbf{c} = \mathbf{H}\mathbf{y}$$
  $\mathbf{H} = \begin{bmatrix} h_{11} & h_{12} & h_{13} & h_{14} \\ h_{21} & h_{22} & h_{23} & h_{24} \end{bmatrix}$ 

## **Optimal measurement combination**

$$\Delta c = h_1 \Delta y_1 + h_2 \Delta y_2 + \dots = H \Delta y$$

• Candidate measurements (y): Include also inputs u



## **Nullspace method**

#### Theorem

Given a sufficient number of measurements ( $n_y \ge n_u + n_d$ ) and no measurement noise, select **H** such that

$$HF = 0$$

where

$$\mathbf{F} = \frac{\partial \mathbf{y}^{opt}}{\partial \mathbf{d}}$$

- Controlling  $\mathbf{c} = \mathbf{H}\mathbf{y}$  to zero yields locally zero loss from optimal operation.

Proof: Given 
$$\partial y^{opt} = F \partial d$$
, and  $c = Hy$ :  $\partial c^{opt} = H \partial y^{opt} = HF \partial d$ 

To make  $\partial c^{opt} = 0$  for any  $\partial d$ , we must have HF = 0.

# Nullspace method (HF=0): Analytic expression for H and proof that it gives J<sub>u</sub>=0

$$J_{u} = J_{uu} \Delta u + J_{ud} \Delta d = [J_{uu} J_{ud}] \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix}$$
$$\Delta y = [G^{y} G_{d}^{y}] \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix} = \tilde{G}_{y} \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix} \rightarrow \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix} = \tilde{G}_{y}^{+} \Delta y$$

Formula for F:

$$J_{u}^{opt} = J_{uu} \Delta u^{opt} + J_{ud} \Delta d = 0 \rightarrow \Delta u^{opt} = -J_{uu}^{-1} J_{ud} \Delta d$$
$$\Delta y^{opt} = \tilde{G}_{y} \begin{bmatrix} \Delta u^{opt} \\ \Delta d \end{bmatrix} = \tilde{G}_{y} \begin{bmatrix} -J_{uu}^{-1} J_{ud} \\ I \end{bmatrix} \Delta d$$
$$\rightarrow F = \tilde{G}_{y} \begin{bmatrix} -J_{uu}^{-1} J_{ud} \\ I \end{bmatrix}$$

Let  $H = [J_{uu}J_{ud}]\tilde{G}_y^+$ . We can verify that HF = 0. Therefore,  $J_u = [J_{uu}J_{ud}]\tilde{G}_y^+\Delta y = H\Delta y = \Delta c$ , and thus controlling c ( $\Delta c = 0$ ) leads to  $J_u = 0$ .

 Proof. Appendix B in: Jäschke and Skogestad, "NCO tracking and self-optimizing control in the context of real-time optimization", Journal of Process Control, 1407-1416 (2011)

# **Example. Nullspace Method for Marathon runner**

```
u = power, d = slope [degrees]

y_1 = hr [beat/min], y_2 = v [m/s]
```

F = 
$$dy_{opt}/dd = \begin{bmatrix} 0.25 \\ -0.2 \end{bmatrix}$$
  
H =  $[h_1 \ h_2]$   
HF =  $0 \rightarrow h_1 f_1 + h_2 f_2 = 0.25 h_1 - 0.2 h_2 = 0$   
Choose  $h_1 = 1 \rightarrow h_2 = 0.25/0.2 = 1.25$ 

Conclusion: c = hr + 1.25 v

Control c = constant → hr increases when v decreases (OK uphill!)

# Extension: "Exact local method" (with measurement noise)

$$\min_{H} \|J_{uu}^{1/2}(HG^{y})^{-1}H\underbrace{[FW_{d}W_{ny}]}_{Y}\|_{F}$$

General analytical solution ("full" H):

$$H = G^{yT}(YY^T)^{-1}$$

- H is unique, except that it can be premultiplied by any nonsingular matrix.
- No noise  $(W_{ny}=0)$ : Cannot use above analytic expression because  $YY^T$  is then singular, but optimal is clearly HF = 0 (Nullspace method)
  - Assumes enough measurements: #y ≥ #u + #d
  - If "extra" measurements (>) then solution to HF=0 is not unique (but above general solution with noise is unique except for premultiplication)
- No disturbances (W<sub>d</sub>= []) + same noise for all measurements (W<sub>ny</sub>= Y = I):
   Optimal is H=G<sup>yT</sup> ("control sensitive measurements")

### Marathon runner: Exact local method

$$F = \begin{bmatrix} 0.25 \\ -0.2 \end{bmatrix}, W_d = 1, W_{ny} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, G^y = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$Y = \begin{bmatrix} FW_d & W_{ny} \end{bmatrix} = \begin{bmatrix} 0.25 & 1 & 0 \\ -0.2 & 0 & 1 \end{bmatrix}$$

$$H = G^{yT}(YY^T)^{-1} \to H = \begin{bmatrix} 0.989 & 1.009 \end{bmatrix}$$

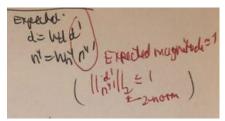
Normalized H1 =  $D^*H = [1 \ 1.02]$ 

Conclusion: c = hr + 1.02 v

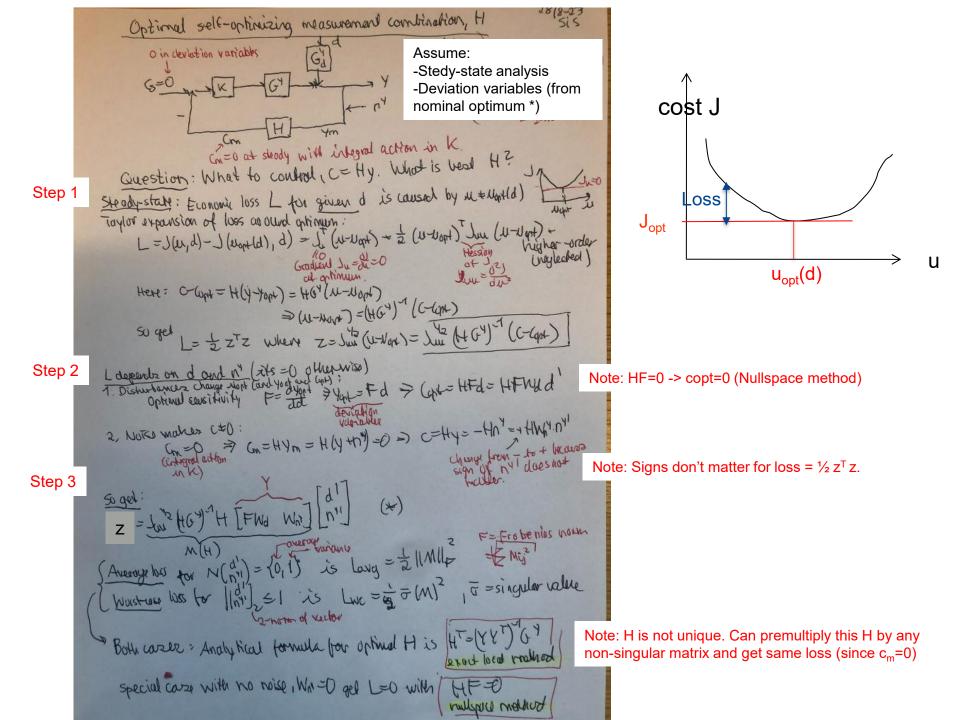
- Before (nullspace method): c = hr + 1.25 v
- Note: Gives same as nullspace when W<sub>ny</sub> is small

### Derivation of «exact local method». 3-steps:

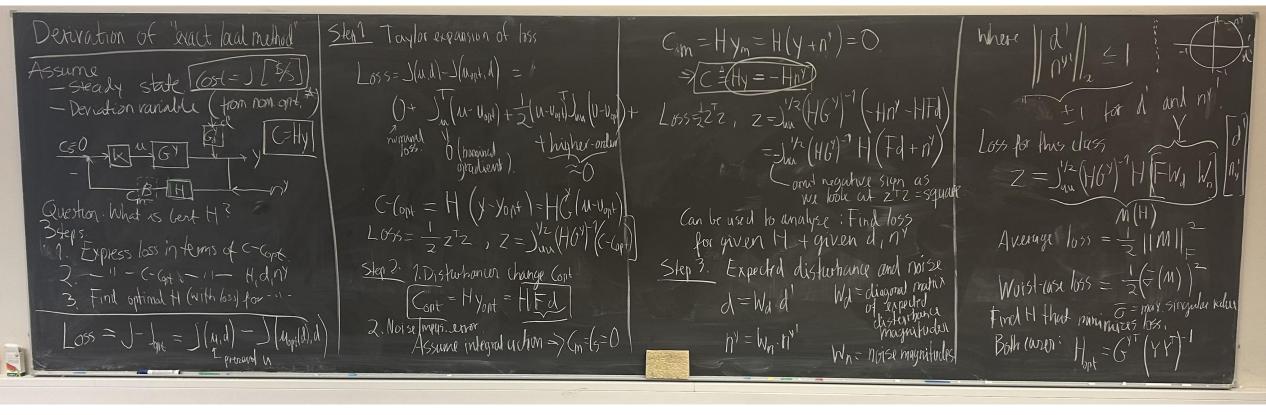
- 1. Express loss in terms of c-c<sub>opt</sub>
- 2. Express c-c<sub>opt</sub> in terms of H, d and n<sup>y</sup>
- 3. Find optimal H (min. loss) for expected d and n<sup>y</sup>



W<sub>d</sub> and W<sub>n</sub> are diagonal matrices with expected magnitudes for d and n<sup>y</sup>

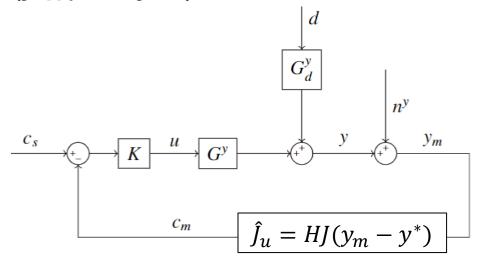


#### From lecture 04 Sep. 2025



# Can use H for static gradient estimation.

$$c_m = \hat{J}_u = H^J(y_m - y^*)$$
. Very simple and works



From «exact local method» of self-optimizing control ( $\tilde{F} \equiv Y$ ):

$$H^{J} = J_{uu} \left[ G^{yT} \left( \tilde{F} \tilde{F}^{T} \right)^{-1} G^{y} \right]^{-1} G^{yT} \left( \tilde{F} \tilde{F}^{T} \right)^{-1}$$
where  $\tilde{F} = [FW_d \ W_{n^y}]$  and  $F = \frac{dy^{opt}}{dd} = G_d^y - G^y J_{uu}^{-1} J_{ud}$ .

- So we premultiply the «simple» H to get the right directions
- and add a constant («bias») which may be viewed as the setpoint c<sub>s</sub>=Hy\*

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Optimal measurement-based cost gradient estimate for feedback real-time optimization

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• Bernardino and Skogestad, Optimal measurement-based cost gradient estimate for real-time optimization, Comp. Chem. Engng., 2024

# **Obtaining F**

F is defined as the gain matrix from the disturbances to the optimal measurements  $\rightarrow \Delta y^{opt} = F \Delta d$ 

Brute force method (often the simplest):

- For every disturbance  $d_i$ ,  $i = 1, ..., n_d$ :
  - Perturb the system with  $\hat{d}_i = d_i + \Delta d_i$ ,  $\Delta d_i$  small
  - Reoptimize the system  $\rightarrow$  obtain change in measurements  $\Delta y^{opt,i}$
  - Obtain *i*-th column of  $F: F_i = \Delta y^{opt,i}/\Delta d_i$
- Return F

### Linearization method for F

*F* can also be obtained from a linearized state-space model:

$$\Delta y = G^{y} \Delta u + G_{d}^{y} \Delta d$$

$$J_{u}(u^{*} + \Delta u, d^{*} + \Delta d) \approx J_{u}^{*} + J_{uu} \Delta u + J_{ud} \Delta d = 0$$

$$\Rightarrow \Delta u^{opt} = -J_{uu}^{-1} J_{ud} \Delta d$$

$$\Delta y^{opt} = G^{y} \Delta u^{opt} + G_{d}^{y} \Delta d = \left(-G^{y} J_{uu}^{-1} J_{ud} + G_{d}^{y}\right) \Delta d$$

$$F = -G^{y} J_{uu}^{-1} J_{ud} + G_{d}^{y}$$

## Toy Example.

$$J = (u - d)^2$$
  
 $n_u = 1$  unconstrained degrees of freedom  
 $u_{\text{opt}} = d$ 

Alternative measurements:

$$y_1 = 0.1(u - d)$$

$$y_2 = 20u$$

$$y_3 = 10u - 5d$$

$$y_4 = u$$

Scaled such that:

$$|d| \leq 1$$
,  $|n_i| \leq 1$ , i.e. all  $y_i$ 's are  $\pm 1$ 

Nominal operating point:

$$d = 0 \Rightarrow u_{\text{opt}} = 0, y_{\text{opt}} = 0$$

What variable c should we control?

#### Single measurements

$$L_{wc} = \frac{1}{2} \ \overline{\sigma} (M)^{2}$$

$$M = J_{uu}^{\frac{1}{2}} (HG^{y})^{-1} H Y,$$

$$Y = [FW_{d} W_{ny}], F = -G^{y} J_{uu}^{-1} J_{ud} + G_{d}^{y}$$

#### . Exact evaluation of loss:

$$L_{wc,1} = 100$$
  
 $L_{wc,2} = 1.0025$   
 $L_{wc,3} = 0.26$   
 $L_{wc,4} = 2$ 

Here: 
$$W_d=1$$
,  $W_{ny}=1$ ,  $J_{uu}=2$ ,  $J_{ud}=-2$ , For  $y_1$ :  $HG^y=0.1$ ,  $HG_d^y=-0.1$ ,  $F=0$ ,  $HY=[0\ 1]$ ,  $M=\sqrt{2}\cdot 10\cdot [0\ 1]$ ,  $L_{wc}=\frac{1}{2}$   $\overline{\sigma}(M)^2=100$  For  $y_2$ :  $HG^y=20$ ,  $HG_d^y=0$ ,  $F=20$ ,  $HY=[20\ 1]$ ,  $M=\sqrt{2}\cdot \frac{1}{20}\cdot [20\ 1]$ ,  $L_{wc}=\frac{1}{2}$   $\overline{\sigma}(M)^2=1.0025$  For  $y_3$ :  $HG^y=10$ ,  $HG_d^y=-5$ ,  $F=-15$ ,  $HY=[5\ 1]$ ,  $M=\sqrt{2}\cdot \frac{1}{10}\cdot [5\ 1]$ ,  $L_{wc}=\frac{1}{2}$   $\overline{\sigma}(M)^2=0.26$ 

# Toy Example. Exact local method. Combine all measurements

$$J = (u - d)^2$$
  
 $n_u = 1$  unconstrained degrees of freedom  
 $u_{\rm opt} = d$ 

Alternative measurements:

$$y_1 = 0.1(u - d)$$
$$y_2 = 20u$$
$$y_3 = 10u - 5d$$
$$y_4 = u$$

Scaled such that:

$$|d| \leq 1$$
,  $|n_i| \leq 1$ , i.e. all  $y_i$ 's are  $\pm 1$ 

Nominal operating point:

$$d = 0 \Rightarrow u_{\text{opt}} = 0, y_{\text{opt}} = 0$$

What variable c should we control?

$$Y = [FW_d W_{ny}],$$
  

$$F = -G^y J_{uu}^{-1} J_{ud} + G_d^y$$
  

$$H = (YY^T)^{-1} G^y$$

Here: 
$$W_d = 1$$
,  $W_{ny} = I$  (4x4),  $J_{uu} = 2$ ,  $J_{ud} = -2$ ,  $G^y = \begin{bmatrix} 0.1 & 20 & 10 & 1 \end{bmatrix}'$ ,  $G_d^y = \begin{bmatrix} -0.1 & 0 & -5 & 0 \end{bmatrix}'$ ,  $F = \begin{bmatrix} 0 & 20 & 5 & 1 \end{bmatrix}'$ ,  $Y = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 20 & 0 & 1 & 0 & 0 \\ 5 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{bmatrix}$ 

$$H = (YY^T)^{-1} G^y = [0.1000 -1.1241 4.7190 -0.0562]$$

Normalized to have 2-norm = 1.

$$H = [0.0206 -0.2317 0.9725 -0.0116]$$

# Toy Example: Nullspace method (not unique)

$$c = Hy = (h_1 \ h_2 \ h_3 \ h_4) \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = h_1y_1 + h_2y_2 + h_3y_3 + h_4y_4$$

#### **B1.** Nullspace method

Neglect measurement error (n = 0):

$$HF = 0$$

Sensitivity matrix

$$\Delta y_{\text{opt}} = F\Delta d; F = (0 \quad 20 \quad 5 \quad 1)^T$$

To find H that satisfies HF = 0 must combine at least two measurements:

$$n_y \ge n_u + n_d = 1 + 1 = 2$$

# Toy Example. Nullspace method with 2 measurements

#### C. Optimal combination

Need two measurements. Best combination is  $y_2$  and  $y_3$ :

$$\begin{pmatrix} y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 20 & 0 \\ 10 & -5 \end{pmatrix} \begin{pmatrix} u \\ d \end{pmatrix}; \ \underline{\sigma} = 4.45$$

Optimal sensitivity:

$$y_{\text{opt}} = Fd; F = \begin{pmatrix} 20\\5 \end{pmatrix}$$

Optimal combination:

$$HF = 0 \Rightarrow (h_1 \quad h_2) \begin{pmatrix} 20 \\ 5 \end{pmatrix} = 0 \Rightarrow 20h_1 + 5h_2 = 0$$

Select 
$$h_1 = 1$$
. Get  $h_2 = -20h_1/5 = -4$ , so

$$c_{\text{opt}} = y_2 - 4y_3$$

Check: 
$$c = y_2 - 4y_3 = 20u - 40u + 20d = -20(u - d)$$
  
(OK!)

## Example where nullspace method «fails»

```
u= reflux
d=feed rate

J = (u-d)<sup>2</sup>
y1 = 0.01(u-d) % temperature product (very small gain!)
y2 = u-0.8d % tempereture inside column
uopt = d
y1opt = 0
y2opt = 0.2 d

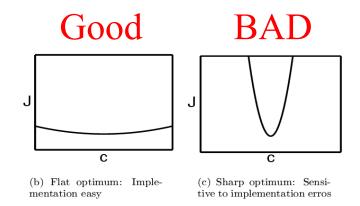
Nullspace: H0=[1 0] % Not good! Use only y1
Exact local method: H=[1 96] % Use y2 instead
```

```
F =[0 0.2]'
Wd=1*eye(1)
Wn=1*eye(2)
Gy = [0.01 1]'
H0=null(F'); H0=H0'/H0(1) % nullspace method
Y = [F*Wd Wn],
H1 = Gy' * inv(Y * Y')
H = H1/H1(1) % exact local method
```

### Conclusion: GOOD "SELF-OPTIMIZING" CV = c

- 1. Optimal value  $c_{opt}$  is constant (independent of disturbance d):
  - $\rightarrow$  Want small optimal sensitivity:  $F_c = \frac{\Delta c_{opt}}{\Delta d} = HF$
- 2. c is "sensitive" to input u (MV) (to reduce effect of measurement noise)
  - $\rightarrow$  Want large gain  $G = HG^y = \frac{\Delta c}{\Delta u}$

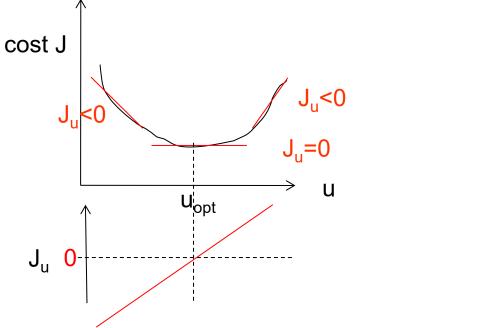
(Equivalently: Optimum should be flat!)



## Optimal steady-state operation with constraints

```
min_u J(u,d)
s.t. g(u,d) \ge 0 (constraints)
```

- J = economic cost [\$/s]
- Unconstrained case: Optimal to keep gradient J<sub>u</sub> = ∂J/∂u =0



Constrained case: KKT-conditions: Active constraints: g=0,

Remaining conconstrained DOFs:  $L_u = J_u + \lambda^T g_u = 0$ 

### WITH CONSTRAINTS

Want tight control of active constraints for economic reasons

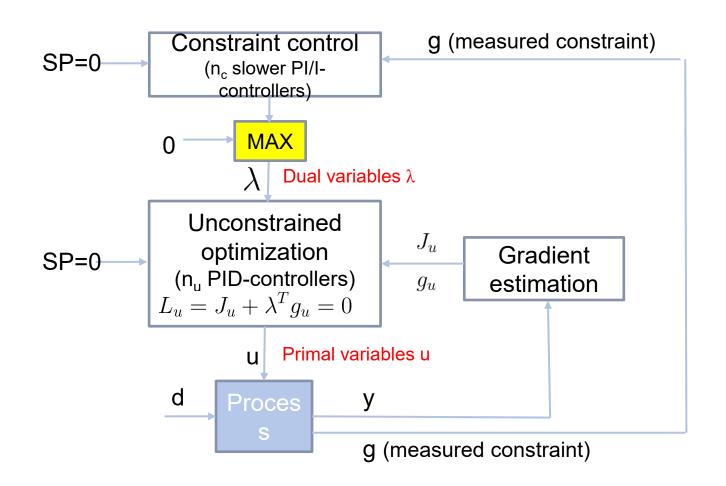
- Active constraint: g<sub>A</sub>=0
- Tight control of g<sub>A</sub> minimizes «back-off»
- How can we identify and control active constraints?
- How can we switch constraints?
- How do find the correct gradient when the constraints change?
- How to implement in the control system?
  - We published 3 approaches in JPC in 2024
  - All may use the «unconstrained» gradient estimate presented above:

$$\hat{J}_u = HJ(y_m - y^*)$$

## I. Primal-dual control based on KKT conditions: Feedback

solution that automatically tracks active constraints by adjusting Lagrange

multipliers (= shadow prices = dual variables)  $\lambda$ 



$$L_u = J_u + \lambda^T g_u = 0$$

Inequality constraints:  $\lambda \geq 0$ 

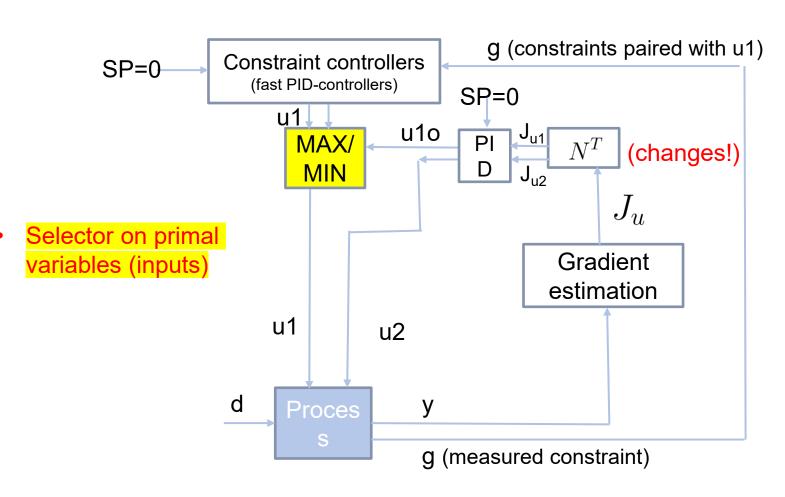
#### Primal-dual feedback control.

- Makes use of «dual decomposition» of KKT conditions
- Selector on dual variables λ
- Problem: Constraint control using dual variables is on slow time scale (can avoid with override)



- D. Krishnamoorthy, A distributed feedback-based online process optimization framework for optimal resource sharing, J. Process Control 97 (2021) 72–83,
- R. Dirza and S. Skogestad. Primal-dual feedback-optimizing control with override for real-time optimization. J. Process Control, Vol. 138 (2024), 103208.

# II. Region-based feedback solution with «direct» constraint control (for case with more inputs than constraints)



 $\mathbf{KKT:} L_u = J_u + \lambda^T g_u = 0$ 

Introduce N:  $N^T g_u = 0$ 

#### Control

- 1. Reduced gradient  $N^T J_u = 0$ 
  - «self-optimizing variables»)
- 2. Active constraints  $g_A = 0$ .

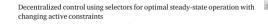
Problem: Simple switching requires at least as many MVs (u) as constraints

Jaschke and Skogestad, «Optimal controlled variables for polynomial systems». S., J. Process Control, 2012

D. Krishnamoorthy and S. Skogestad, «Online Process Optimization with Active Constraint Set Changes using Simple Control Structure», I&EC Res., 2019

Bernardino and Skogestad, Decentralized control using selectors for optimal steady-state operation with changing active constraints, J. Process Control, Vol. 137, 2024





## III. Region-based MPC with switching of cost function (for general case)

#### Standard MPC with fixed CVs: Not optimal

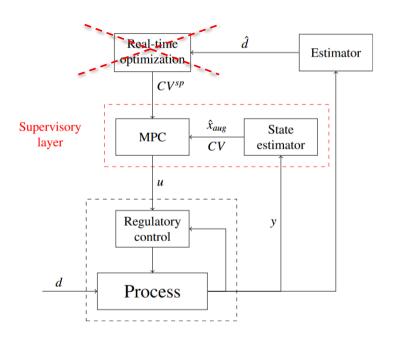


Figure 1: Typical hierarchical control structure with standard setpoint-tracking MPC in the supervisory layer. The cost function for the RTO layer is  $J^{ec}$  and the cost function for the MPC layer is  $J^{MPC}$ . With no RTO layer (and thus constant setpoints  $CV^{sp}$ ), this structure is not economically optimal when there are changes in the active constraints. For smaller applications, the state estimator may be used also as the RTO estimator.

$$J^{MPC} = \sum_{k=1}^{N} ||CV_k - CV^{sp}||_Q^2 + ||\Delta u_k||_R^2$$

#### Proposed: With changing cost (switched

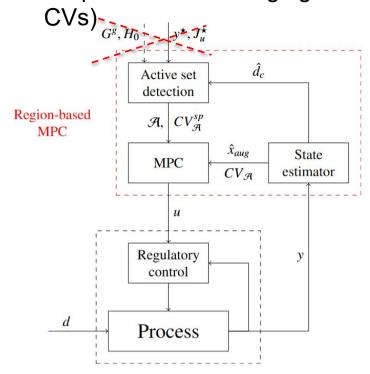


Figure 2: Proposed region-based MPC structure with active set detection and change in controlled variables. The possible updates from an upper RTO layer  $(y^*, J_u^* \text{ etc.})$  are not considered in the present work. Even with no RTO layer (and thus with constant setpoints  $CV_{\mathcal{A}}^{sp}$ , see (14) and (15), in each active constraint region), this structure is potentially economically optimal when there are changes in the active constraints.

changes in the active constraints.
$$J_{\mathcal{A}}^{MPC} = \sum_{k=1}^{N} \|CV_{\mathcal{A}} - CV_{\mathcal{A}}^{sp}\|_{Q_{\mathcal{A}}}^{2} + \|\Delta u_{k}\|_{R_{\mathcal{A}}}^{2}$$

$$CV_{\mathcal{A}} = \begin{bmatrix} g_{\mathcal{A}} \\ c_{\mathcal{A}} \end{bmatrix} = \begin{bmatrix} g_{\mathcal{A}} \\ N_{\mathcal{A}}^{T} H_{0} y \end{bmatrix}$$

$$H_{0} = \begin{bmatrix} J_{uu} & J_{ud} \end{bmatrix} \begin{bmatrix} G^{y} & G_{\mathcal{A}}^{y} \end{bmatrix}^{\dagger}$$

$$M_{0} = \begin{bmatrix} J_{uu} & J_{ud} \end{bmatrix} \begin{bmatrix} G^{y} & G_{\mathcal{A}}^{y} \end{bmatrix}^{\dagger}$$

$$M_{0} = \begin{bmatrix} J_{uu} & J_{ud} \end{bmatrix} \begin{bmatrix} G^{y} & G_{\mathcal{A}}^{y} \end{bmatrix}^{\dagger}$$

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