# Self-optimizing control Theory – including constraints

«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\*:

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

subject to:

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

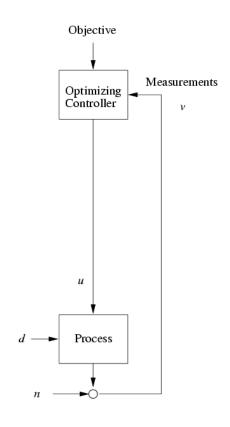
Operational constraints: g(u, x, d) < 0

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

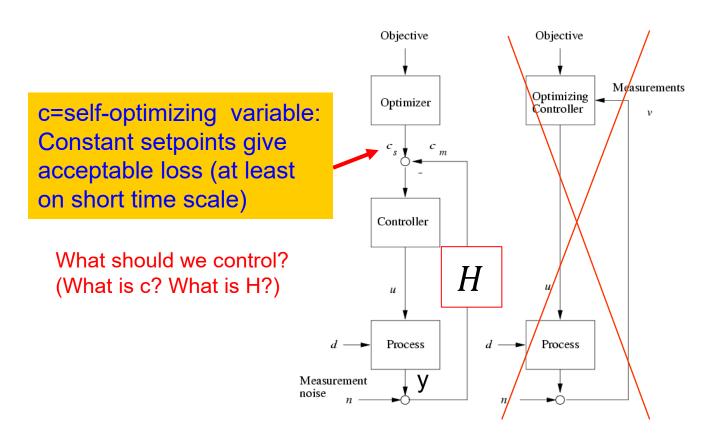
How should we adjust the degrees of freedom (u)?

What should we control?

# "Optimizing Control" (EMPC)



## "Self-Optimizing Control"



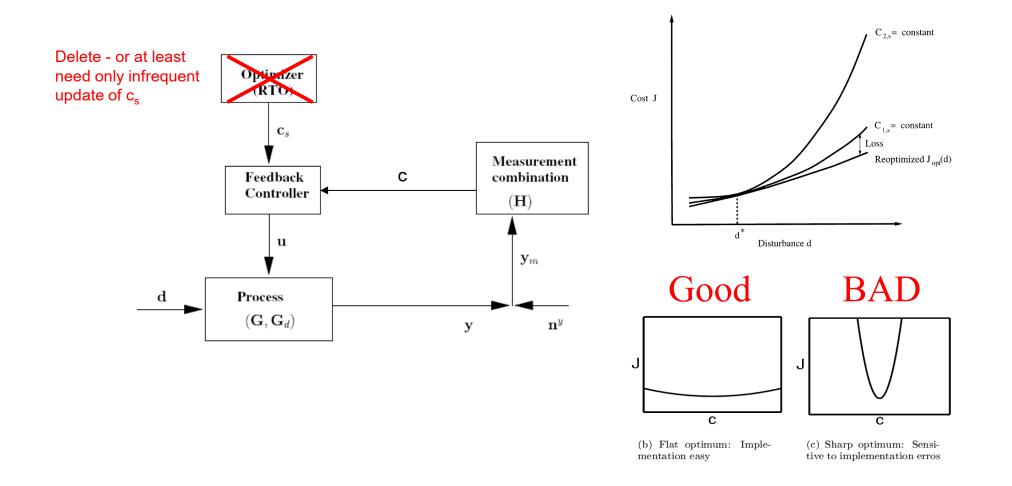
c = Hy

#### *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?



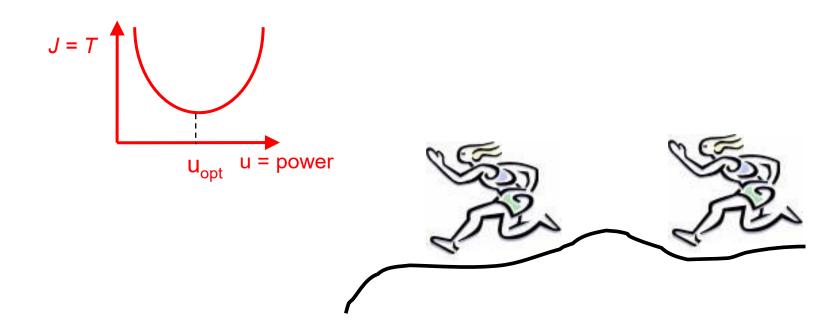
## 1. Sprinter case

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



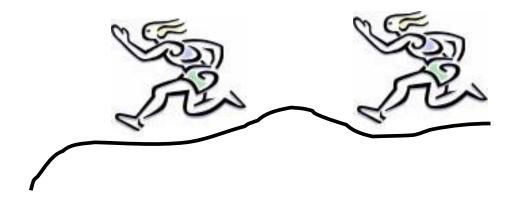
### 2. Marathon runner case

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

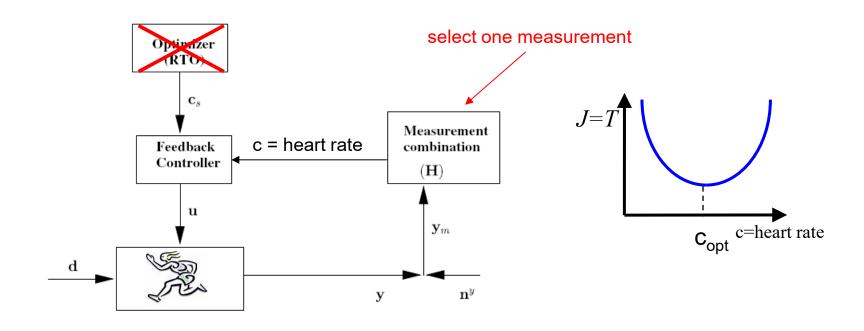


## Self-optimizing control: Marathon

- 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**

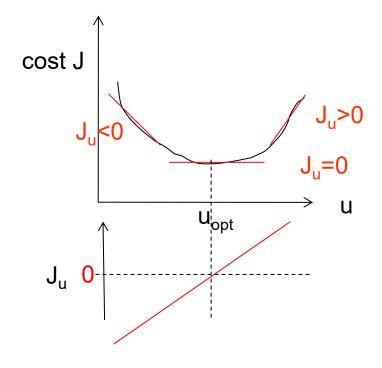


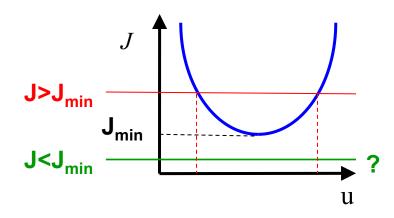
- CV = heart rate is good "self-optimizing" variable
- Simple and robust implementation
- Disturbances are indirectly handled by keeping a constant heart rate
- May have infrequent adjustment of setpoint (c<sub>s</sub>)

# 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





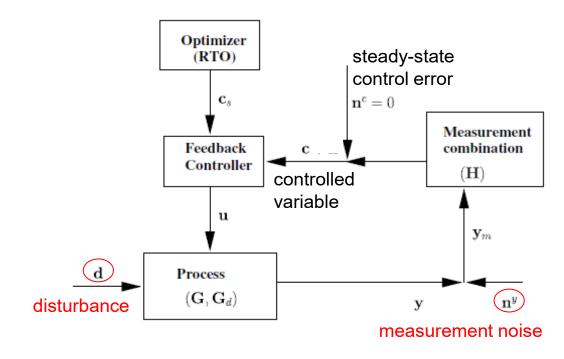
# Unconstrained optimum: **NEVER** try to control a variable that reaches max or min at the optimum

- 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<sub>min</sub>: 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:

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

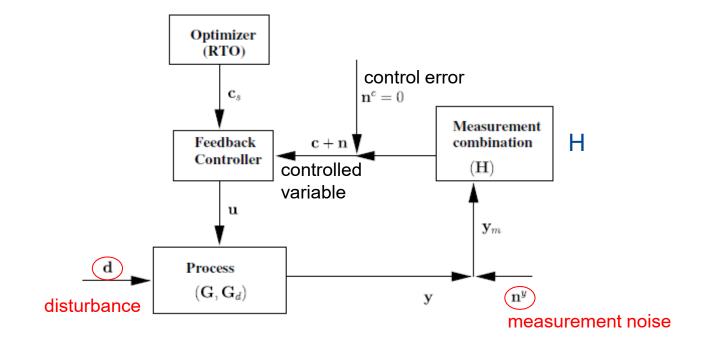
Combinations of measurements:

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

## **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)

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

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")
    - Proof: Use analytic solution

### Marathon runner: Exact local method

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

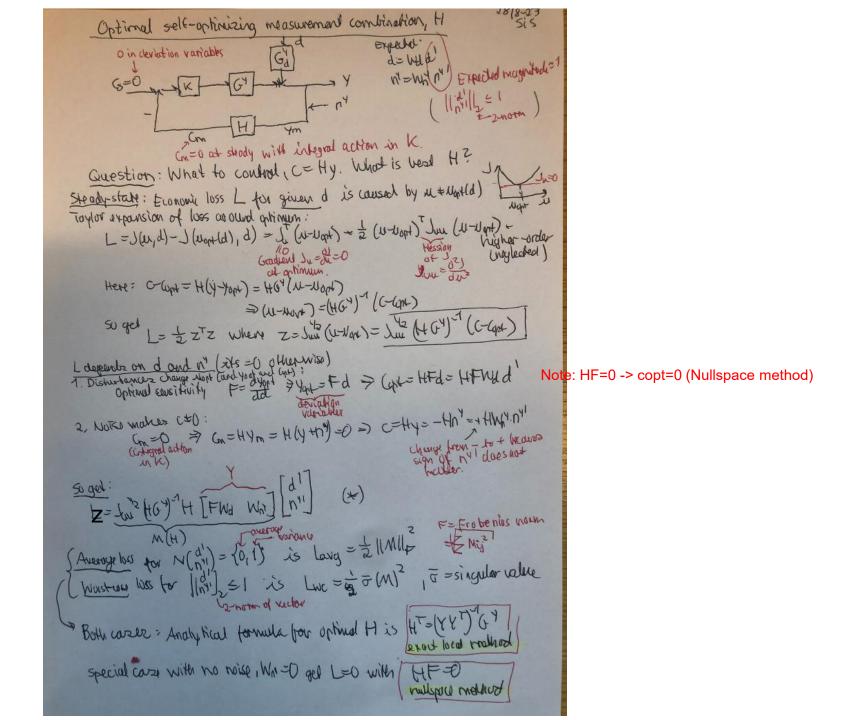
$$Y = \begin{bmatrix} FW_d & W_{ny} \end{bmatrix} = \begin{bmatrix} 0.25 & 1 & 0 \\ -0.2 & 0 & 1 \end{bmatrix}$$

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

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

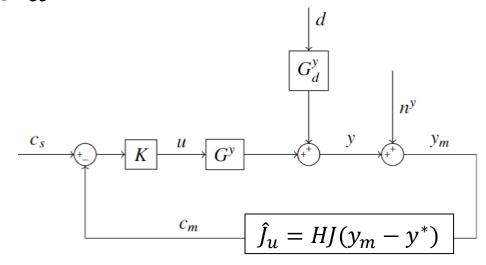
Conclusion: c = hr + 1.02 v

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



# Can use for static gradient estimation.

 $c_m = \widehat{J}_u$ . Very simple and works well!



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 «previous» 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  $u_{
m opt}=d$ 

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  $y_1$ :  $HG^y=0.1$ ,  $HG_d^y=-0.1$ ,  $F=0$ ,  $F$ 

# Toy Example. Exact local method. Combine all measurements

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

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

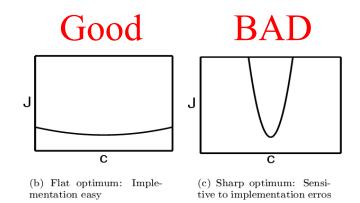
Nullspace: H0=[1 0] % Not good! Use only y1
Exact local method: H=[1 96] % Use y2 instead
```

```
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  $G = HG^y = \frac{\Delta c}{\Delta u}$

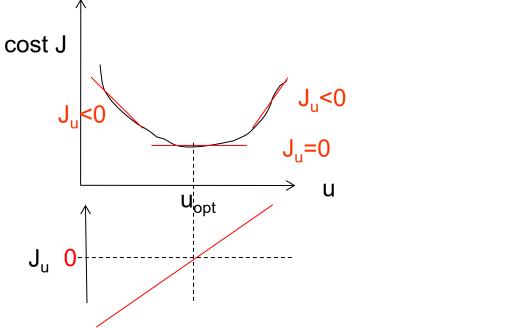
(Equivalently: Optimum should be flat!)



## 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

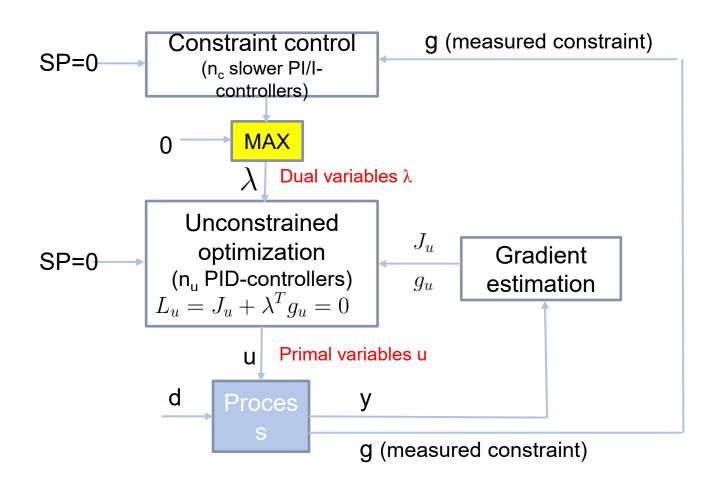
- Active constraint: g<sub>A</sub>=0
- Tight control of g<sub>A</sub> minimizes «back-off»
- How can we identify and control active constraints?
- How can we switch constraints?
- How do find the correct gradient when the constraints change?
- How to implement in the control system?
  - We published 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:  $\lambda \geq 0$ 

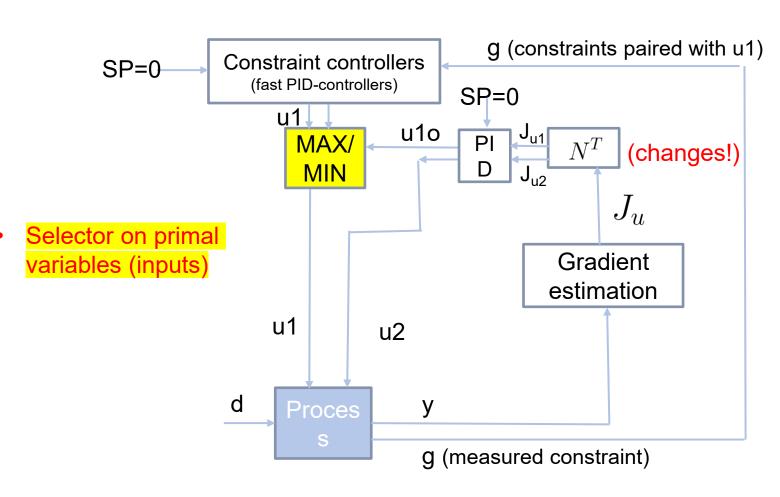
#### Primal-dual feedback control.

- Makes use of «dual decomposition» of KKT conditions
- Selector on dual variables λ
- Problem: Constraint control using dual variables is on slow time scale



- 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 constrints  $g_{\Delta} = 0$ .



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

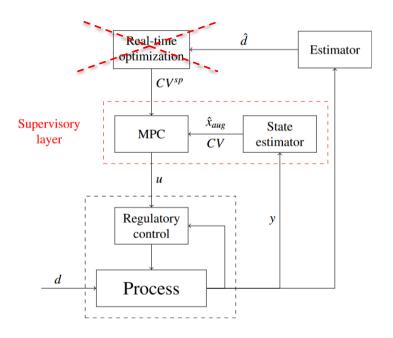


Figure 1: Typical hierarchical control structure with standard setpoint-tracking MPC in the supervisory layer. The cost function for the RTO layer is  $J^{ec}$  and the cost function for the MPC layer is  $J^{MPC}$ . With no RTO layer (and thus constant setpoints  $CV^{sp}$ ), this structure is not economically 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

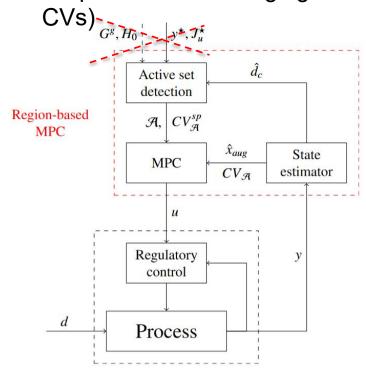


Figure 2: Proposed region-based MPC structure with active set detection and change in controlled variables. The possible updates from an upper RTO layer  $(y^*, J_u^* \text{ etc.})$  are not considered in the present work. Even with no RTO layer (and thus with constant setpoints  $CV_{\mathcal{A}}^{sp}$ , 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.
$$J_{\mathcal{A}}^{MPC} = \sum_{k=1}^{N} \|CV_{\mathcal{A}} - CV_{\mathcal{A}}^{sp}\|_{Q_{\mathcal{A}}}^{2} + \|\Delta u_{k}\|_{R_{\mathcal{A}}}^{2} \qquad CV_{\mathcal{A}} = \begin{bmatrix} g_{\mathcal{A}} \\ c_{\mathcal{A}} \end{bmatrix} = \begin{bmatrix} g_{\mathcal{A}} \\ N_{\mathcal{A}}^{T} H_{0} y \end{bmatrix}$$

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

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

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

