Advanced Process Control and Global Optimization for Complex Processes



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Research Scope



Outline



PART I : Model Predictive Control for Nonlinear ODE System

Model Predictive Control



Refinery





Artificial Pancreas



Semiconductor Manufacturing

Pharmaceutical Manufacturing

Nonlinear Model Predictive Control



Feedforward

Robust Stability

• Robust control Lyapunov function (RCLF: $V(x) = x^T P x$)



Robust Control Lyapunov Function

Objective: Enlarging ROA and reducing residual set

Characterize the level of ROA

 $\max_{P} \left(\frac{\min_{\overline{x}} \overline{x}^{T} P \overline{x}}{\max_{\hat{x}} \hat{x}^{T} P \hat{x}} \right)$ Characterize the level of residual set s.t. $\inf_{u} \sup_{\Delta f, \Delta g} \overline{x}^{T} P \cdot \left(f(\overline{x}) + \Delta f + \left(g(\overline{x}) + \Delta g \right) u \right) \ge 0$

$$u_{\min} \le u \le u_{\max}$$
$$P \succ 0$$

 $\hat{x} \in \Omega$

$$\overline{x}^T P \overline{x} \ge \max_{\hat{x} \in \Omega} \hat{x}^T P \hat{x}$$

Bilevel Optimization:

Fractional programming: Dinkelbach's method **Coordinate search: Single variable optimization**

Yang & Lee, IET control theory and application, 2012 Yang & Lee, Journal of Process Control, 2011

Performance Improvement

Approximate Dynamic Programming



MPC:
$$u(k), u(k+1), \cdots, u(k+p)$$

H. Nosair, Y. Yang & J. M. Lee, Control Engineering Practice, 2010 Y. Yang & J. M. Lee, Computers and Chemical Engineering, 2010



Uncertainty $\dot{C}_{A} = \frac{F}{V} \Big(C_{A0} (1 + \varepsilon) - C_{A} \Big) - k_{0} e^{-E/RT_{R}} C_{A} \quad \text{Uncertainty}$ $\dot{T}_{R} = \frac{F}{V} \Big(T_{R0} - T_{R} \Big) - \frac{\Delta H}{\rho C_{p}} k_{0} e^{-E/RT_{R}} C_{A} + \frac{Q_{\sigma}}{\rho C_{p} V} + \mu$ 402 400 398 396 **MPC ADP** ⊢[∞] 394 8.6s 0.1s Average computational time 392 390 252.7 230.2 Average control cost 388 $\sum_{k=p}^{k+p} \left(x(t) - x_{\text{setpoint}} \right)^{\mathrm{T}} Q\left(x(t) - x_{\text{setpoint}} \right)$

Y. Yang & J. M. Lee, Journal of Process Control, 2012 Y. Yang & J. M. Lee, Journal of Process Control, 2013



PART II : Advanced Process Control for PDE System

PDE Control: Motivation







Heat equation

Fluid mechanics

Rod pump



Crystallization



Lithium battery

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Engine

PDE Control: Application



Stress difference Hooke's law *z*: position Friction

t: time

Sensor: Surface

Estimation:

Downhole load & Displacement







PDE Control: Application

Displacement and load estimation: Proposed method Proposed method Classical mathod Classical method 10 1.8 1.6 Displacement (Feet) Dynamic load (Lbs) **Downhole Displacement** 1.4 1.2 Downhole Load 0.8 0.6 0 0.4 2 3 6 7 8 9 10 0 4 5 2 3 9 n 4 5 6 7 8 Time (s) Time (s) x 10 12 2.2 Classical method Classical method Proposed method Proposed method 10 1.8 Displacement (Feet) 1.6 Dynamic load (Lbs) 1.4 1.2 0.8 2

0.6

0.4 L

1

2

3

4

5

Time (s)

6

7

8

9

10

(Y. Yang & S. Dubljevic, SPE Annual Conference, 2012)

8

9

10

7

0

2

3

4

5 6

Time (s)

10

PDE Control: Model Reduction

	Spectr	al method:		Slow modal state
$x(z,t) = \sum_{i=1}^{\infty} a_i(t)\phi_i(z) -$			$\underbrace{\text{Truncation}}_{x(z,t)} \approx \sum_{i=1}^{n_s} a_i(t) \phi_i(z)$	
	State #	FD 2 nd order (max error)	FD 4 th order (max error)	Fourier spectral (max error)
	16	6.13e-1	2.36e-1	2.55e-4
	32	1.99e-1	2.67e-2	1.05e-11
	64	5.42e-2	1.85e-3	6.22e-13

My theoretical contributions:

Handle the truncation residual in the model predictive control

$$x(z,t) = \sum_{i=1}^{n_s} a_i(t)\phi_i(z) + R(z,t)$$

Controller and observer synthesis by taking residual into account

Spectral Methods in Fluid Dynamics, Canuto, 1988 (Table 1.1 1st order wave equation). 15

PDE Control: Model Predictive Control

Two-phase flow (linearized K-S equation)



 $\frac{\partial x}{\partial t} + v \frac{\partial^4 x}{\partial \zeta^4} + \frac{\partial^2 x}{\partial \zeta^2} = 0,$ $x(0,t) = 0, x(l,t) = d_1 u(t) + d_2 \mu(t),$ x(0,t) = 0, x(l,t) = u(t), $u(t), \mu(t): \text{ boundary inputs,}$ $x(\zeta,t): \text{ variance of the thin film thickness.}$

Spectral method Galerkin's model reduction MPC (Full state feedback)

(Y. Yang & S. Dubljevic, Journal of process control, 2013)

PDE Control: Controller & Observer

• Controller and observer synthesis: $\hat{a}_{u}(k+1) = \Lambda_{u}\hat{a}_{u}(k) + \mathfrak{B}_{u}\tilde{u}(k) + L_{u}(y(k) - y_{s}(k) - \hat{y}_{u}(k))$ $a_{s}(k+1) = \Lambda_{s}a_{s}(k) + \mathfrak{B}_{s}\tilde{u}(k)$ $\tilde{u}(k+1) = K_{u}\hat{a}_{u}(k) + G_{u}u(k)$ $a = \begin{bmatrix} a_{1}, a_{2}, \cdots, a_{n_{u}}, | a_{n_{u}+1}, a_{n_{u}+2}, \cdots, a_{n_{u}+n_{s}}, a_{n_{u}+n_{s}+1}, a_{n_{u}+n_{s}+2}, \cdots \end{bmatrix}$ Slow modal states *Questions*

- 1. How to find the order of slow modal states?
- 2. How to design the feedback law and observer gains to obtain a closed-loop system with large enough region of attraction?

PDE Control: Controller & Observer

Results (2nd order Parabolic PDE Stabilization)



(Y. Yang & S. Dubljevic, European journal of control, 2014)

PART III : Global Optimization under Uncertainty



Massachusetts Institute of Technology



Motivation







Refinery

Metabolic network



 $\min_{x,y} c^{\mathrm{T}}x$

s.t. $Ax \leq b$,

 $F(x, y) \leq d$, $x \in \Re, y \in \{0,1\}.$

Global Optimization: mixed-integer nonlinear programming (MINLP)

Overview

Refinery Optimization under Uncertainty



 Objective: decide the optimal crude oil procurement and refinery operations to maximize the profit, meet market demands and satisfy quality specifications.
 (U.S. Patent Pub. No: US2016/0140448 A1)

Model 1



• Blending & Splitting (Pooling problem) $z = x \cdot y$

J. P. Favennec, Refinery operation and management, Editions TECHNIP, 2001

Model 1: Uncertainties

Uncertainties:

Crude	VR yield	Sulfur	
Skarv	10.3%	0.209%	
Saturno	26.7%	0.373%	
Plutonio	21.6%	0.2%	hility
Brent	13.6%	0.253%	Proha
Hungo	25.5%	0.321%	
Polvo	37.2%	0.741%	
Zakum	10.9%	0.966%	
Basra	26.2%	1.826%	
Thunder	20.1%	0.416%	
Mars	27.6%	1.216%	

Crude oil yields: www.bp.com

Gaussian Distribution: Mean=nominal value Standard deviation=0.1×nominal value



Sampling: 120 scenarios with different VR yield & sulfur content

Solution: Stochastic Programming

Stochastic programming vs. Deterministic method:

Deterministic method: $x_d^* = \max_{x_d} - \text{Cost}(x_d) + \text{Profit}_{\text{Nominal}}(x_d)$

Stochastic method: $x_s^* = \max_{x_s} -\operatorname{Cost}(x_s) + \sum_i \operatorname{Profit}_i(x_s) \cdot \operatorname{Pr}_i$

Solution: Stochastic Programming

Two-stage Stochastic Formulation (Model 1):

min cost of crude oil purchase

s.t. Crude oil source restrictions,

10 Crude oil

Discretization of each crude oil quantity: 5000 barrels = 1 lot

 Model (120 scenarios): 13061 constraints, 100 binary variables 13800 continuous variables 2760 bilinear terms

(Yang & Barton, AIChE Journal, 2016)

E (product sales – operation costs)
Material balance,
Unit capacity limits,
Demand requirements,
Quality constraints,
Pooling equations

120 Scenarios: different VR yields and sulfur concentration

We use the non-convex generalized Benders decomposition (NGBD).

Method: NGBD

Results: Profit/Time

	GAMS ¹	C++ ²	(BARON, Antigone)
Total time	12.2 hours	10 mins	No solution in 1 day

1. General Algebraic Modeling System (GAMS)

2. Joint work with Rohit Kannan.

Model 2: Flowchart

J. P. Favennec, Refinery operation and management, Editions TECHNIP, 2001

◆ Decision variables: cut point temperature $T_j \in [\underline{T}_j, \overline{T}_j]$

- $P_{\text{dis,VR}}$: Total mole flowrate in the distillate of VR cut
- $P_{\text{bot,VR}}$: Total mole flowrate in the bottom (yield) of VR cut.

A. M. Alattas, I. E. Grossmann and I. Palou-Rivera, I&EC research, 2011, 2012.

Fractionation index (FI) equation

 $\frac{\mathcal{X}_{\mathrm{dis},j,i}}{\mathcal{X}_{\mathrm{dis},j,i}} = \left(K_{j,i}\left(T_{j}\right)\right)^{FI}$ $x_{\text{dis.} i,i}$: Mole fraction of pseudocomponent i in the distillate of cut j $x_{\text{bot, } j, i}$: Mole fraction of pseudocomponent *i* in the bottom of cut *j* $FI = \begin{cases} FI_{r,j} & \text{if } T_{j,\text{ini}} \leq Tb_i < T_j \\ FI_{r,j} & \text{if } T_{j,\text{ini}} \geq Tb_i \geq T_j \end{cases}, \quad Tb_i: \text{ true boiling point of pseudocomponent } i \end{cases}$ $= \left(K_{j,i} \left(T_{j} \right) \right)^{FI_{r,j}} v_{i} + \left(K_{j,i} \left(T_{j} \right) \right)^{FI_{s,j}} \left(1 - v_{i} \right), \quad v_{i} \in \{0,1\},$ $K_{j,i}(T_j) = \frac{\operatorname{VP}_i(T_j)}{P}$, VP: vapor pressure, K: equilibrium constant

Gilbert, R.J.H., AIChE Journal, 1966.

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Model 2: Uncertainty

Uncertainty is in the heavy part of true boiling point (TBP) curve

Solution: Stochastic Programming

Two-stage Stochastic Formulation (Model 2):

min cost of crude oil purchase + \mathbb{E} (operation costs – product sales)

s.t. Crude oil source restrictions,

4 Crude oil

Discretization of each crude oil quantity: 5000 barrels = 1 lot Material balance, Unit capacity limits, CDU model, Demand requirements, Quality constraints, Pooling equations

- Model (16 scenarios):
 - 10058 constraints,

168 binary variables (128 in CDU model)

- 8452 continuous variables
- 8032 bilinear terms

3456 signomial terms: $K(T_j)^7 = K(T_j)^{6.9} = K(T_j)^{4.25}$

Nominal Scenario

Difficult global optimization problem (ANTIGONE)

Optimization: NGBD

Comparison

Computational time

Time/Iterations	Adaptive ¹	Non-adaptive ²
PBP (s)	3932	3896
Dual-PBP-PCR (s)	41572	87009
PP (s)	10686	6094
RMP (s)	148	73
Total time (h)	15.6	26.9
Iteration	126	95

- 1. Add binary variable if relaxation gap >=10%.
- 2. Use 6 binary variables for piecewise relaxation .

Results:

Summary

 Research Scope: Advanced process control/Scheduling for complex processes under uncertainties

 Methods: MPC, reinforcement learning, spectral method, two-stage stochastic programming (NGBD).

 Applications: Rod pump, refining process design, CSTR control

Supplement

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PDE Control: Model Reduction

Parabolic PDE (Example: 2nd order)

$$\frac{\partial x(z,t)}{\partial t} = b \frac{\partial^2 x(z,t)}{\partial z^2} + c \frac{\partial x(z,t)}{\partial z} + dx$$
$$y_c(t) = \int_0^1 x(z,t) \delta(z-z_c) dz$$
$$Point-wise output$$

Eigenfunction analysis

$$\mathfrak{A} \coloneqq b \frac{\partial^2}{\partial z^2} + c \frac{\partial}{\partial z} + d$$

Solve $\mathfrak{A}z = \lambda_i \phi_i(z)$
Let $f_i(z) = \phi_i(z)$, then
 $x(z,t) \approx \sum_{i=1}^{n_s} a_i(t) \phi_i(z)$

Boundary condition

$$x(0,t) = u(t), \quad \frac{\partial x(1,t)}{\partial z} = 0$$

 $x(z,0) = x_0(t)$ Initial condition
 $|\dot{u}(t)| \le 15$ Input constraint

PDE Control: Model Reduction

Decomposition & Boundary transformation:

PDE Control: MMPC

Modal model predictive control:

(Assume x(z,t) can be measured) $\longrightarrow a_u, a_s$ are known in real time $\min_{u,\mu} \int_{t=0}^{t_{T}} y_{s}^{T} Q y_{s} + u^{T} W_{1} u + \mu^{T} W_{2} \mu$ s.t. $\dot{a}_{s} = \Lambda_{s} a_{s} + B_{1s} u + B_{2s} \mu$, Control performance • Output for unstable $\dot{a}_{\mu} = \Lambda_{\mu}a_{\mu} + B_{\mu}u + B_{\mu}\mu,$ modal states $y_{u} = Ca_{u}\phi_{u} + B_{1u}\dot{u} + B_{2u}\dot{\mu}, \qquad y = x(z_{c},t) \text{ output}$ $y_s = Ca_s\phi_s + B_{1s}\dot{\mu} + B_{2s}\dot{\mu},$ $y_{\min} \leq y_s + y_f + y_\mu \leq y_{\max},$ $|u| \leq \overline{u}, \quad |\mu| \leq \overline{\mu}, \quad a_{s} \cup a_{\mu} \in \mathbb{R}^{7},$ $\left| y_{f} \right| \leq C \overline{a}_{f} \overline{\phi}_{f} + \overline{B}_{1f} \overline{\dot{u}} + \overline{B}_{2f} \overline{\dot{\mu}}$ • Static bound of the output for fast modal states

PDE Control: Controller & Observer

• Dynamic upper and lower bounds for: $y_f(k)$

 $\tilde{y}_{f}\left(k+1\right)^{-} \leq y_{f}\left(k+1\right) \leq \tilde{y}_{f}\left(k+1\right)^{+}$

PDE Control: Controller & Observer

• Solve linear matrix inequality (LMI): K_u, G_u, L_u

$$\begin{vmatrix} S_1 & 0 & \left[K_u, G_u\right]^{\mathrm{T}} \\ 0 & S_2 & -K_u^{\mathrm{T}} \\ \left[K_u, G_u\right] & -K_u & \dot{u}_{\max}^2 I \\ \Xi_1^{\mathrm{T}} S \Xi_1 - S \prec 0, \quad \Xi_2^{\mathrm{T}} S \Xi_2 - S \prec 0. \end{vmatrix} \succ 0,$$

where

$$\Xi_{1} = \begin{bmatrix} \overline{\Lambda}_{u} & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \begin{bmatrix} K_{u}, G_{u} \end{bmatrix} & -\begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \begin{bmatrix} K_{u}, G_{u} \end{bmatrix} & -\begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \begin{bmatrix} K_{u}, G_{u} \end{bmatrix} & -\begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \begin{bmatrix} K_{u}, G_{u} \end{bmatrix} & -\begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \begin{bmatrix} K_{u}, G_{u} \end{bmatrix} & -\begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \begin{bmatrix} K_{u}, G_{u} \end{bmatrix} & -\begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \begin{bmatrix} K_{u}, G_{u} \end{bmatrix} & -\begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \begin{bmatrix} K_{u}, G_{u} \end{bmatrix} & 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\overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix} \end{bmatrix} = \begin{bmatrix} \overline{\mathfrak{B}}_{u} \\ \Lambda \end{bmatrix}$$

Convergence: $\lim_{k \to \infty} x(z,k) \to 0.$ **Feasibility:** LMI is guaranteed to be feasible by increasing the dimension of a_s

Pseudocomponent method:

Optimization: Range Reduction

Optimization: Relaxation

Convex/Piecewise convex relaxation

Optimization: Piecewise Relaxation

How to select the partition variable/point to get tighter cutting plane?

Optimization: Local Cutting Plane

- Objective: design the dual cutting plane only valid in a specific region $\left[\underline{c}_{p}, \overline{c}_{p}\right]$.
- Benefits:

Note:
$$c_p = \left(20d_p + \sum_{t=1}^{9} 2^{t-1}D_{p,t}\right)Q\rho_p$$

1. Better bounds for convex relaxation.

$$f_{p,i} = y_{p,i}c_p, \ c_p \in \left[\underline{c}_p, \overline{c}_p\right] \Longrightarrow f_{p,i} \in \left[\underline{y}_{p,i}\underline{c}_p, \ \overline{y}_{p,i}\overline{c}_p\right]$$

2. Extra tight constraints for Dual-PBP-PCR.

$$\sum_{i \in \Omega} f_{p,i} = c_p, \ c_p \in \left[\underline{c}_p, \overline{c}_p\right] \Longrightarrow \sum_{i \in \Omega} f_{p,i} \in \left[\underline{c}_p, \ \overline{c}_p\right]$$

Optimization: Local Cutting Plane

• Enhanced PBP-PCR/Dual-PBP-PCR $\min_{x,\delta,y,f,b} w(x_s)$

s.t. $\sum_{k \in \Omega} f_{p,k,s} = \left(20d_p^* + \sum_{t=1}^9 2^{t-1}D_{p,t}^* \right) Q\rho_p,$ $\sum_{k \in \Omega} f_{p,k,s} \in \left[\underline{c}_p, \ \overline{c}_p\right],$ $G(x_s, y_{p, i, s}, f_{p, i, s}, \delta_s) \leq 0,$ $b_{p,i,j,s} \ge \overline{f}_{p,j,s} y_{p,i,s} + f_{p,j,s} \overline{y}_{p,i,s} - \overline{f}_{p,j,s} \overline{y}_{p,i,s},$ $b_{p,i,j,s} \ge f_{p,j,s} y_{p,i,s} + f_{p,j,s} y_{p,i,s} - f_{p,j,s} y_{p,i,s},$ $b_{p,i,j,s} \leq \overline{f}_{p,j,s} y_{p,i,s} + f_{p,j,s} y_{p,i,s} - \overline{f}_{p,j,s} y_{p,i,s},$ $b_{p,i,j,s} \leq \underline{f}_{p,j,s} y_{p,i,s} + f_{p,j,s} \overline{y}_{p,i,s} - f_{p,j,s} \overline{y}_{p,i,s},$ $\sum_{i\in\Omega} b_{p,i,j,s} = f_{p,j,s}, \qquad \sum_{i\in\Omega} b_{p,i,j,s} = f_{p,i,s},$ $\{x_s, y_{n,i,s}, f_{n,i,s}\} \in \Pi_s, \ \delta_s \in \{0,1\}^n,$ $i \in \Omega, j \in \Omega, p \in \Theta$.

$$\begin{split} \min_{\delta,y,f,b} & w(x_s) + \sum_{\forall p \in \Theta} \lambda_{s,p} \left(\sum_{k \in \Omega} f_{p,k,s} - \left(20d_p^* + \sum_{t=1}^9 2^{t-1} D_{p,t}^* \right) Q\rho_p \right) \\ \text{s.t. } G\left(x_s, y_{p,j,s}, f_{p,i,s}, \delta_s \right) &\leq 0, \quad \sum_{k \in \Omega} f_{p,k,s} \in \left[\underline{c}_p, \ \overline{c}_p \right], \\ b_{p,i,j,s} &\geq \overline{f}_{p,j,s} y_{p,i,s} + f_{p,j,s} \overline{y}_{p,i,s} - \overline{f}_{p,j,s} \overline{y}_{p,i,s}, \\ b_{p,i,j,s} &\geq f_{p,j,s} y_{p,i,s} + f_{p,j,s} \underline{y}_{p,i,s} - f_{p,j,s} \underline{y}_{p,i,s}, \\ b_{p,i,j,s} &\leq \overline{f}_{p,j,s} y_{p,i,s} + f_{p,j,s} \overline{y}_{p,i,s} - \overline{f}_{p,j,s} \overline{y}_{p,i,s}, \\ b_{p,i,j,s} &\leq f_{p,j,s} y_{p,i,s} + f_{p,j,s} \overline{y}_{p,i,s} - f_{p,j,s} \overline{y}_{p,i,s}, \\ b_{p,i,j,s} &\leq f_{p,j,s} y_{p,i,s} + f_{p,j,s} \overline{y}_{p,i,s} - f_{p,j,s} \overline{y}_{p,i,s}, \\ \sum_{i \in \Omega} b_{p,i,j,s} &= f_{p,j,s}, \quad \sum_{j \in \Omega} b_{p,i,j,s} = f_{p,i,s}, \\ \left\{ x_s, y_{p,i,s}, f_{p,j,s} \right\} \in \Pi_s, \ \delta_s \in \{0,1\}^n, \\ i \in \Omega, j \in \Omega, p \in \Theta. \end{split}$$

Optimization: Local Cutting Plane

Variables: *d*, *D*

$$\eta_{s} \geq \text{obj}_{\text{Dual-PBP-PCR}}\left(c^{*}\right) + \lambda_{s}^{T}Bc^{*} - 20BQ\sum_{p=1}^{4}\lambda_{p,s}\rho_{p}d_{p} - BQ\sum_{p=1}^{4}\lambda_{p,s}\rho_{p}\sum_{t=1}^{9}2^{t-1}D_{p,t}$$

New cut (local valid):

$$\eta_{s} \geq \operatorname{obj}_{\text{E-Dual-PBP-PCR}}\left(c^{*}\right) + \lambda_{s}^{\mathrm{T}}Bc^{*} - 20BQ\sum_{p=1}^{4}\lambda_{p,s}\rho_{p}d_{p} - BQ\sum_{p=1}^{4}\lambda_{p,s}\rho_{p}\sum_{t=1}^{9}2^{t-1}D_{p,t}$$
$$+ \sum_{p=1}^{4}M_{s}\sum_{h\in\Upsilon, D_{p,h}^{*}=0}D_{p,h} + \sum_{i=1}^{4}M_{s}\sum_{h\in\Upsilon, D_{p,h}^{*}=1}\left(1 - D_{p,h}\right)$$

 $M_s < 0$, can be determined systematically

Note:
$$\operatorname{obj}_{\text{E-Dual-PBP-PCR}}(c^*) \ge \operatorname{obj}_{\text{Dual-PBP-PCR}}(c^*)$$

Optimization: Non-separable case

Bilinear term=stage I variable × stage II variable

