A Discretization-based Approach for Multiperiod Blend Scheduling Problem

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Reference

Today's talk will mainly focus on the following papers:

1. Kolodziej SP, Castro PM, Grossmann IE. Global optimization of bilinear programs with a multiparametric disaggregation technique*. J Glob Optim.* 2013; 57: 1039-1060

A discretization technique for bilinear programs

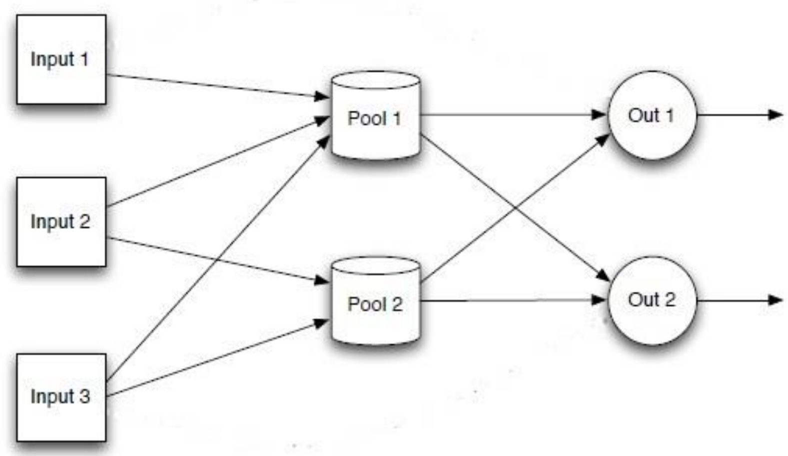
2. Kolodziej SP, Grossmann IE, Furman KC, Sawaya NW. A discretization-based approach for the optimization of the multiperiod blend scheduling problem. *Comput Chem Eng*. 2013; 53: 122–142.

Solution methods for multiperiod blend scheduling problem based on the technique mentioned in previous paper

Introduction

What is Blending

Multiple *streams* with different *properties* are sent to *pools* to produce blend product, the product must satisfy certain property *specifications*.



Industrial Practice Example

Crude Oil Blending:

Streams – Crudes (from Saudi Arabia, North Sea…)

Properties – Sulfur, Specific gravity...

Pools – Charging tanks

Gasoline Blending:

Streams – Fuel Components

Properties – Octane number, Vapor pressure…

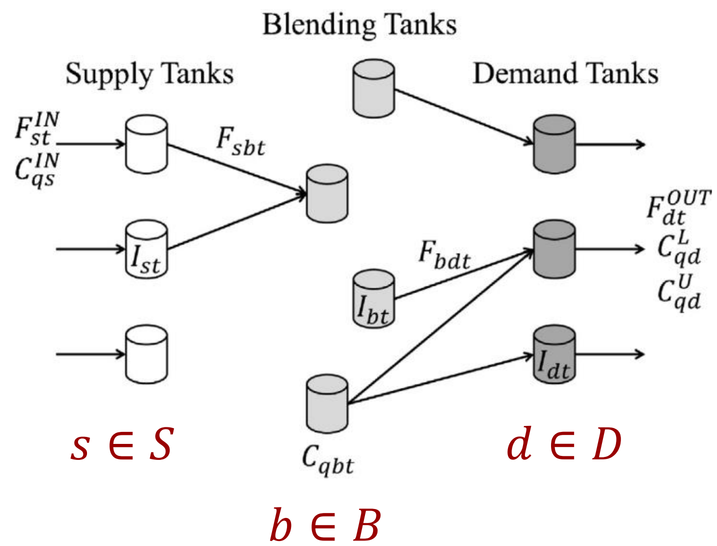
Pools – Blenders

*Misener R, Floudas CA. Advances for the pooling problem: Modeling, global optimization, and computational studies. *Appl Comput Math*, 2009; 8: 3–22.

Problem Statement

Given

- A set of nodes $n \in TA$ consist of subsets of *supply*, *blending* and *demand* tanks $TA = S \cup B \cup D$
- Directed arcs $(n, n') \in N$ connect nodes
- A set of time periods $T = \{0, \dots, t, \dots, H\}$
- A set of properties $q \in Q$
- Incoming supply flows $F_{s,t}^{IN}, s \in S$ at each period, and corresponding property $C_{q,s}^{IN}$
- Demand flows $F_{d,t}^{OUT}, d \in D$ that are withdrawn from demand tanks at each time period
- Property specifications for demand tanks $C_{q,d}^{L}$ and $C_{q,d}^{U}$
- Cost/prices for supply/demand flows β_s/β_d, fixed/variable cost for flows within the network $\alpha_{n,n'}/\beta_{n,n'}$



Determine

Flows between tanks at each time period

Objective

Maximizing profit

Multiperiod Blending Problem(MPBP)

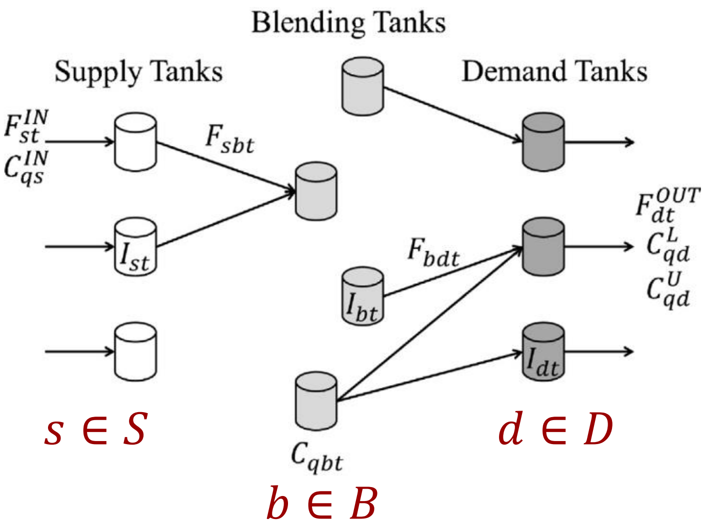
Variables:

$F_{n,n',t}$: Flows from node n to n' at time t

$I_{n,t}$: Inventory level of node n at time t

$C_{q,b,t}$: Property level of q inside node b at time t

$y_{n,n',t}$: Transfer material from node n to n' at time t (*binary*)



Constraints:

$$F_{n,n',t} \le F_{n,n'}^{U} \cdot y_{n,n',t} \quad \forall (n,n') \in N, t \in T$$
$$F_{n,n',t} \ge F_{n,n'}^{L} \cdot y_{n,n',t} \quad \forall (n,n') \in N, t \in T$$

Bounds on flowrates

$$I_{s,t} = I_{s,t-1} + F_{s,t}^{IN} - \sum_{n \in B} F_{s,n,t} \quad \forall s \in S, t \in T$$
$$I_{b,t} = I_{b,t-1} + \sum_{n \in S} F_{n,b,t} - \sum_{n \in D} F_{b,n,t} \quad \forall b \in B, t \in T$$
$$I_{d,t} = I_{d,t-1} + \sum_{n \in B} F_{n,d,t} - F_{d,t}^{OUT} \quad \forall b \in B, t \in T$$

Inventory balance

$$y_{s,b,t} + y_{b,d,t} \le 1$$
$$\forall n \in S, b \in B, d \in D, t \in T$$

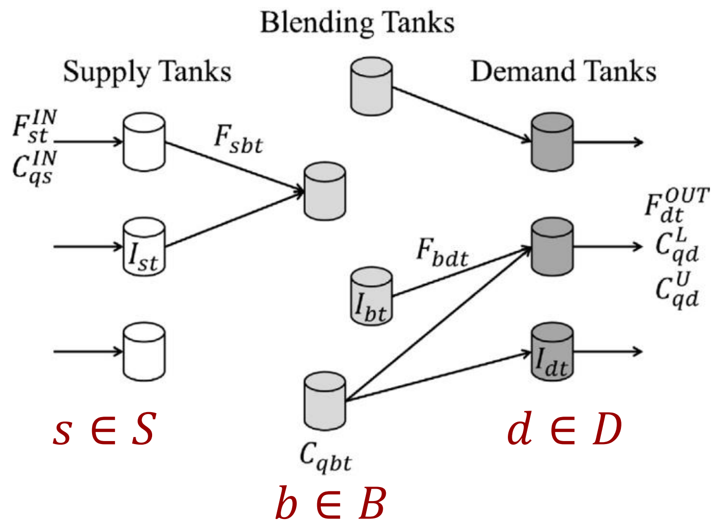
No simultaneously feeding/withdrawing for blending tanks

Model Formulation

Multiperiod Blending Problem(MPBP)

Constraints:

$$C_{q,b,t-1} \leq C^U_{q,d} + M(1 - y_{b,d,t})$$
$$C_{q,b,t-1} \geq C^L_{q,d} + M(1 - y_{b,d,t})$$
$$\forall q \in Q, b \in B, d \in D, t \in T$$



Property specifications

$$I_{b,t}C_{q,b,t} = I_{b,t-1}C_{q,b,t-1} + \sum_{n \in S}(F_{n,b,t} \cdot C^{IN}_{q,s}) - \sum_{n \in D}(F_{b,n,t} \cdot C_{q,b,t-1}) \quad \forall q \in Q, b \in B, t \in T$$

Bilinear terms

Property balance

Objective function

$$max \sum_{t \in T}\left[\sum_{n \in S}\sum_{d \in D}\beta_d F_{n,d,t} - \sum_{s \in S}\sum_{b \in B}\beta_s F_{s,b,t} - \sum_{(nn') \in N}(\alpha_{n,n'} y_{n,n',t} + \beta_{n,n'} F_{n,n',t})\right]$$

Revenue from products

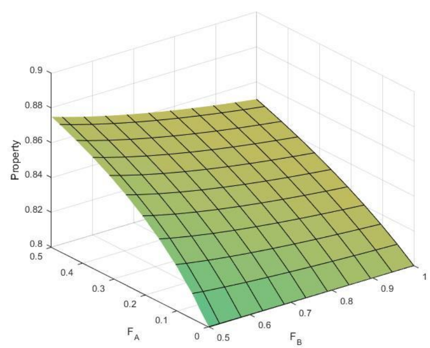
Cost from supply

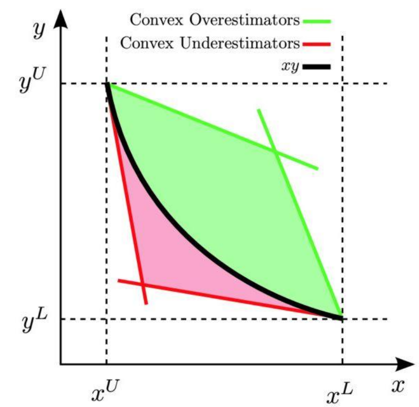
Fixed and variable cost for pumping

Challenges

- Multiperiod Blending Problem(MPBP) is an MINLP
- When the general purpose MINLP solvers attempt to solve it through global optimization techniques, such as spatial B&B, nonlinear constraints will be relaxed:

$$\underline{I_{b,t}C_{q,b,t}} = I_{b,t-1}C_{q,b,t-1} + \sum_{n\in S}(F_{n,b,t}\cdot C_{q,s}^{IN}) - \sum_{n\in D}(F_{b,n,t}\cdot C_{q,b,t-1}) \quad \forall q\in Q, b\in B, d\in D, t\in T$$





McCormick Envelop

$$\underline{w = xy}$$
$$w \ge x^L y + x y^L - x^L y^L$$
$$w \ge x^U y + x y^U - x^U y^U$$
$$w \le x^L y + x y^U - x^L y^U$$
$$w \le x^U y + x y^L - x^U y^L$$

- Property balance can be violated in the relaxed problem
- The nature of the objective function incentivizes the solver to exploit the gap between the original formulation and the relaxation, results in *off-spec* products

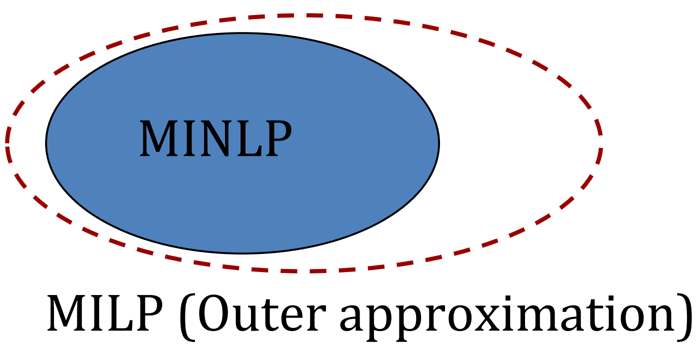
*McCormick G. Computability of global solutions to factorable nonconvex programs: Part i - convex underestimating problems. *Math Program*. 1976; 10: 147-175

Proposed Approach

Traditional techniques:

Construct an MILP, that is necessarily feasible, assuming an MINLP solution exist

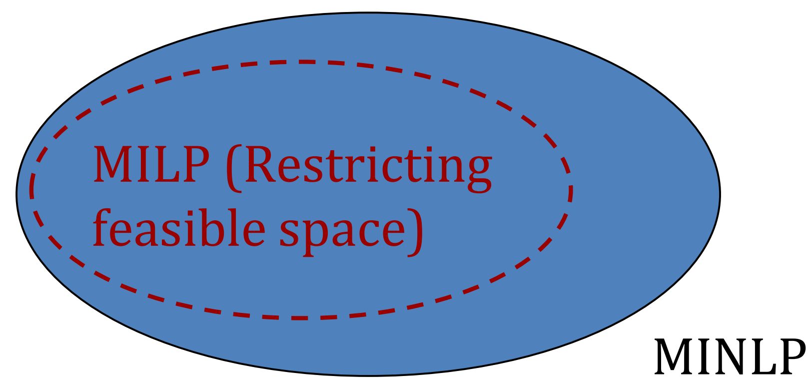
Solvers struggle to find the feasible solutions to the MINLP problem



Proposed technique:

Construct an MILP, that is necessarily MINLP feasible, assuming an MILP solution exist

Solution to the MILP, is guaranteed to be feasible in the MINLP



Remark:

The MILP approximation is constructed in a conceptually different manner

Radix-based Discretization

For *any positive real number x*, we have

$$x = \sum_{l \in \mathbb{Z}} \sum_{k=0}^{R-1} R^l \cdot k \cdot y_{k,l}$$

R: Numerical base
k: Digits in base R
l : Power

For *decimal* system:
$R = 10, k = \{0,1,2,\ldots,9\}$
For *binary* system:
$R = 2, k = \{0,1\}$

$$y_{k,l} = \begin{cases} 1 & \text{If the digit } k \text{ take the place at } R^l \\ 0 & \text{Otherwise} \end{cases}$$

Exactly *one* digit can take the place at R^l

$$\sum_{k=0}^{R-1} y_{k,l} = 1, \forall l \in \mathbb{Z}$$

Example(decimal):

$$x = 3.1 = 3 \times 10^0 + 1 \times 10^{-1}$$
$$y_{3,0} = 1, y_{1,-1} = 1$$

Discretization and Approximation

The exact representation of x may require infinitively many terms

$$x = \sum_{l \in \mathbb{Z}} \sum_{k=0}^{R-1} R^l \cdot k \cdot y_{k,l}$$

Summation over an *infinite* set

By specifying the upper/lower bounds of the power l, we approximate the value of x

$$x = \sum_{l=p}^{P} \sum_{k=0}^{R-1} R^l \cdot k \cdot y_{k,l}$$

Summation over an *finite* set

Example(decimal) :

$R = 10, k = \{0,1,2, \dots, 9\}$

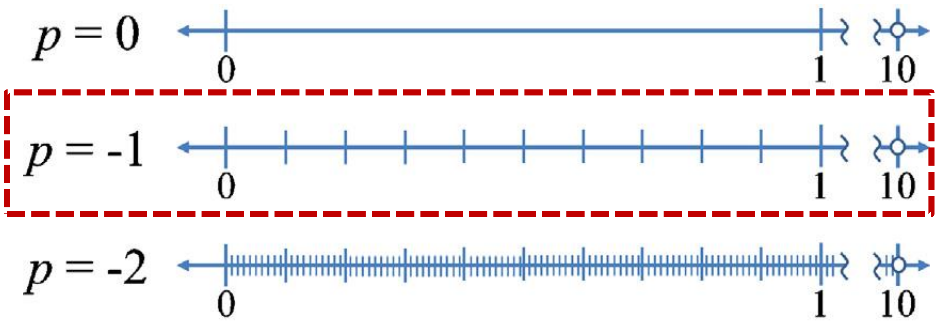
If we pick , $p = P = 0$

$x = \{0,1,2,3,\dots,9\}$ → x *cannot* be 3.14159….

Discretization and Approximation

Discretized axes using radix-based (base 10) discretization for $P = 0, p = \{0, -1, -2\}$

$$x = \sum_{l=p}^{P} \sum_{k=0}^{R-1} R^l \cdot k \cdot y_{k,l}$$



Characteristics of radix-based (base 10) discretization at $P = 0, p = \{0, -1, -2\}$

p (smallest power)	0	−1	−2
P (largest power)	0	0	0
Range	0–9	0–9.9	0–9.99
Increment	1	0.1	0.01
Significant digits	1	2	3
Binary variables (RBD)	10	20	30
Binary variables (traditionally)	10	100	1000

Remark:

Suppose $x \in [1,10]$, after discretization, the feasible space is restricted

Discretization for Bilinear Terms

$$\underline{I_{b,t}C_{q,b,t}} = \underline{I_{b,t-1}C_{q,b,t-1}} + \sum_{n\in S}(F_{n,b,t}\cdot C_{q,s}^{IN}) - \sum_{n\in D}\underline{(F_{b,n,t}\cdot C_{q,b,t-1})} \quad \forall q\in Q, b\in B, t\in T$$

Two types of bilinear terms: $I\cdot C$ and $F\cdot C$

The authors decided to discretize property level C

$$C_{q,b,t} = \sum_{l=p}^{P}\sum_{k=0}^{9} 10^l\cdot k\cdot z_{k,l,q,b,t} \quad \forall q\in Q, b\in B, t\in T$$

$$W_{q,b,t}^{IC} = \underline{I_{b,t}C_{q,b,t}} = \sum_{l=p}^{P}\sum_{k=0}^{9} 10^l\cdot k\cdot \underline{I_{b,t}\cdot z_{k,l,q,b,t}} \quad \forall q\in Q, b\in B, t\in T$$

Bilinear term

Bilinear term, product of one *continuous* variable and one *binary* variable

Let $\hat{I}_{k,l,q,b,t} = I_{b,t}\cdot z_{k,l,q,b,t}$ we have

$$\hat{I}_{k,l,q,b,t} \le I_b^U\cdot z_{k,l,q,b,t} \quad \forall l,k,q,b,t$$

$$\sum_{k=0}^{9}\hat{I}_{k,l,q,b,t} = I_{b,t} \quad \forall l\in\{p,\ldots,P\}, q, b, t$$

Exact linearization(Oral and Kettani, 1992)

Oral M, Kettani O. A linearization procedure for quadratic and cubic mixed-integer problems. *Oper Res.*1992; 40(Suppl 1): S109–S116

Discretization for Bilinear Terms

1. Discretize property level C

$$C_{q,b,t} = \sum_{l=p}^{P} \sum_{k=0}^{9} 10^l \cdot k \cdot z_{k,l,q,b,t} \quad \forall q \in Q, b \in B, t \in T$$

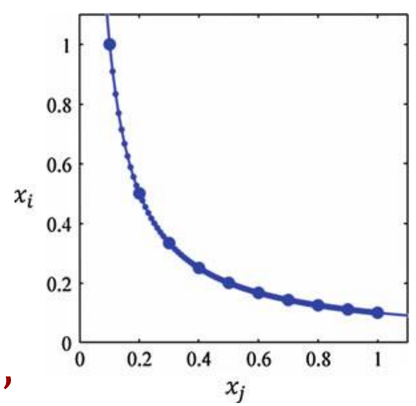
2. Rewrite bilinear term $I \cdot C$ and $F \cdot C$

$$W_{q,b,t}^{IC} = I_{b,t} C_{q,b,t} = \sum_{l=p}^{P} \sum_{k=0}^{9} 10^l \cdot k \cdot I_{b,t} \cdot z_{k,l,q,b,t} = \sum_{l=p}^{P} \sum_{k=0}^{9} 10^l \cdot k \cdot \hat{I}_{k,l,q,b,t} \; \forall q \in Q, b \in B, t \in T$$

$$W_{q,b,n,t}^{FC} = F_{b,n,t} C_{q,b,t} = \sum_{l=p}^{P} \sum_{k=0}^{9} 10^l \cdot k \cdot F_{b,n,t} \cdot z_{k,l,q,b,t} = \sum_{l=p}^{P} \sum_{k=0}^{9} 10^l \cdot k \cdot \hat{F}_{k,l,q,b,n,t} \; \forall q \in Q, b \in B, t \in T$$

3. Rewrite bilinear constaints with $W_{q,b,t}^{IC}$ and $W_{q,b,n,t}^{FC}$

$$W_{q,b,t}^{IC} = W_{q,b,t-1}^{IC} + \sum_{n \in S} (F_{n,b,t} \cdot C_{q,s}^{IN}) - \sum_{n \in D} W_{q,b,n,t}^{FC} \quad \forall q \in Q, b \in B, t \in T$$



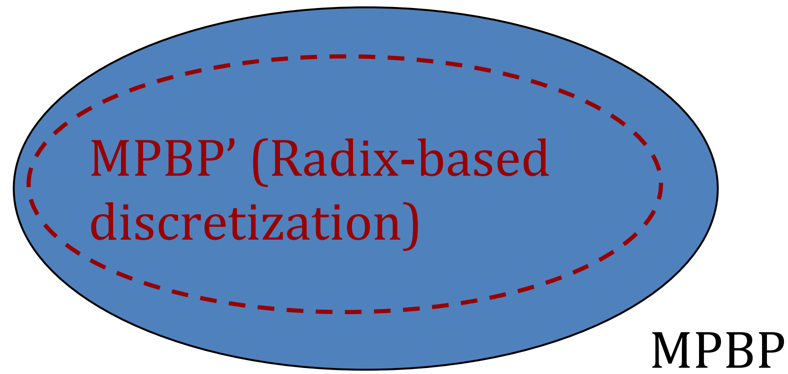
By doing so ,we restrict the feasible space of the original problem. We denote the new problem as MPBP'

Heuristic 1

Multiperiod blending problem(MPBP): MINLP

After discretization (MPBP’): MILP

The solution of MPBP’ is guaranteed to be *feasible* in MPBP



Heuristic 1

Step 0. Choose power p, P for discretization

Step 1. Solve MPBP’ to obtain an *approximation* of the solution z’

Step 2. Fix binary variables in MPBP to the values found by solving MPBP’, solve MPBP (now *NLP*)

Step 3. Optionally, set $p = p - 1$, return to step 1

Shortcomings:

- Lacks termination criteria
- Cannot guaranteed global optimality
- No information about gaps

Computational Results

7 MPBP Instances solved by BARON

Table 5
Results of BARON for 7 different instances ofmultiperiod blendproblems.

Tanks	6	8	8	8	8	8	8
Time periods	3	3	3	3	4	4	4
Qualities	2	2	2	2	2	2	2
Wall time (s)	21.12	>7200	>7200	>7200	>7200	>7200	>7200
Relative gap	52.3%	23.7%	205.6%	13.4%	13.4%	409.5%	17.2%
Constraints	214	625	607	628	861	885	737
Continuous variables	67	136	136	136	185	189	169
Binary variables	36	87	87	87	120	124	104
Non-zero elements	543	1722	1672	1766	2413	2469	2107
Nonlinear non-zeros	64	256	244	256	376	376	358

Same instances solved using Heuristic 1

Obj. found by BARON = 13.1040

Global Optimal = 13.5268

Table 8
Computational results for Heuristic 1.

Tanks	6	8	8	8	8	8	8
Time periods	3	3	3	3	4	4	4
Total wall time (s)	9.96	839.0	245.0	250.2	337.3	4800.6	978.5
MILP solve (Gurobi)							
Wall time (s)	9.94	838.8	244.9	250.1	336.9	4800.1	978.1
Objective function	13.3594	45.2554	7.3818	13.5268	53.9496	9.2051	19.9806
Constraints	1886	7089	6811	7092	9557	9581	9083
Continuous variables	1319	4632	4466	4632	6713	6717	6449
Binary variables	420	855	855	855	1144	1148	1128
NLP post-solve (BARON)							
Wall time (s)	0.02	0.16	0.03	0.19	0.32	0.5	0.37
Objective function	13.3594	45.2804	7.3936	13.5268	53.9627	9.2266	20.039
MILP-NLP difference	0.00%	0.06%	0.16%	0.00%	0.02%	0.23%	0.29%
Constraints	215	459	657	579	467	447	633
Continuous variables	131	327	465	419	323	327	457

Upper Bounding

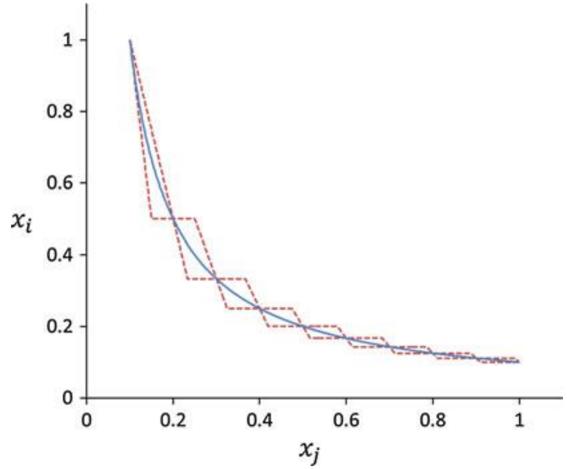
$$C_{q,b,t} = \sum_{l=p}^{P}\sum_{k=0}^{9} 10^l \cdot k \cdot \underbrace{z_{k,l,q,b,t}}_{\text{Binary}} + \sum_{k=0}^{1} 10^p \cdot k \cdot \underbrace{\tilde{z}_{k,l,q,b,t}}_{\text{Continuous}} \quad \forall q \in Q, b \in B, t \in T$$

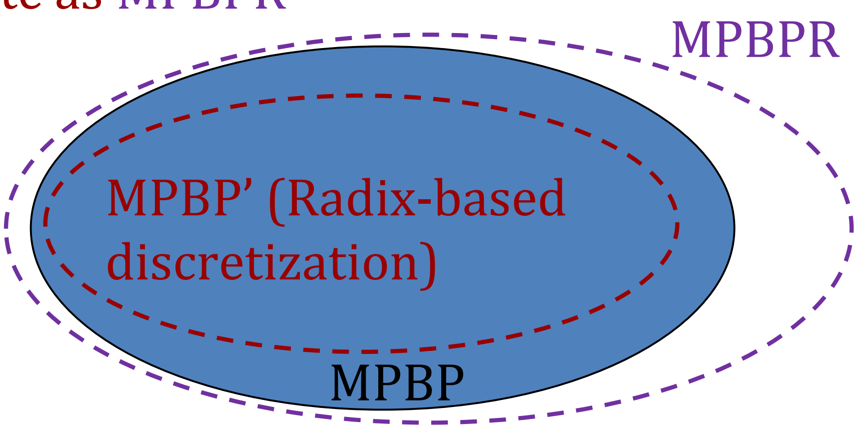
Fill the gap between discretized points

$$W^{IC}_{q,b,t} = I_{b,t}C_{q,b,t} = \sum_{l=p}^{P}\sum_{k=0}^{9} 10^l \cdot k \cdot \hat{I}_{k,l,q,b,t} + \sum_{k=0}^{1} 10^p \cdot k \cdot I_{b,t} \cdot \tilde{z}_{k,l,q,b,t} \quad \forall q \in Q, b \in B, t \in T$$

Bilinear term with two continuous variables

Linearize the bilinear term using outer approximation, we obtain a relaxation of MPBP', denote as MPBPR





Algorithm 1

Algorithm 1

Step 0. Choose power p, P for discretization, set $z^L = -\infty$

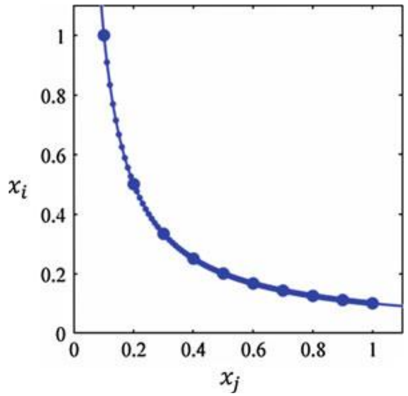
Step 1. Solve MPBPR to obtain the upper bound z^R

Step 2. Solve MPBP' to obtain the lower bound z'. If MPBP' is infeasible, let $z' = -\infty$. Update overall lower bound $z^L = max\{z^L, z'\}$

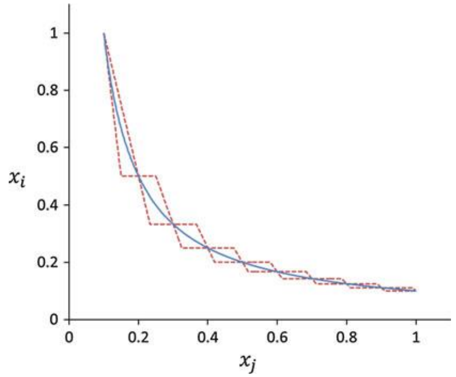
Step 3. If $(z^R - z^L)/z^R \leq \varepsilon$, STOP, global optimal solution found. Otherwise, set $p = p - 1$, return to step 1

Shortcomings:

Need to solve two MILP at each iteration



MPBP'



MPBPR

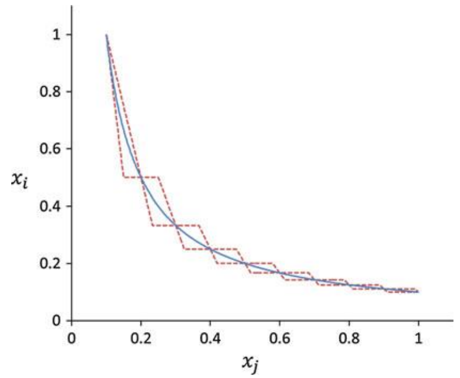
Algorithm 2

Step 0. Choose power p, P for discretization, set $z^L = -\infty$

Step 1. Solve MPBPR to obtain the upper bound z^R

Step 2. Fix binary variables in MPBP to the values found by solving MPBPR, solve MPBP using a local NLP solver with the start point obtained from MPBPR, obtain some lower bound z^L

Step 3. If $(z^R - z^L)/z^R \le \varepsilon$, STOP, global optimal solution found. Otherwise, set $p = p - 1$, return to step 1



MPBPR

Comparison

7 MPBP Instances solved using heuristic 1, algorithm 1 and algorithm 2

Table 11
Comparison of performance between Heuristic 1 and Algorithms 1 and2.

Tanks	6	8	8	8	8	8	8
Time periods	3	3	3	3	4	4	4
Total wall time (s)							
Heuristic 1	9.96	839.0	245.0	250.2	337.3	4800.6	978.5
Algorithm 1	2.17	4573.5	2588.7	426.5	338.7	12,309.0	1525.9
Algorithm 2	3.97	2839.9	120.5	15.5	41.3	2831.1	44.2

Overall algorithm 2 has the best performance

For most instances, MPBP’ is significantly more difficult to solve, compare to MPBPR

Summary

1. Global optimization algorithm based on discretization for multiperiod blend scheduling problem is proposed

2. The discretization technique can be applied to general optimization problem with bilinear terms

Follow up papers:

- Castro PM, Grossmann IE. Global Optimal Scheduling of Crude Oil Blending Operations with RTN Continuous-time and Multiparametric Disaggregation. *Ind Eng Chem Res.* 2014; 53 (39): 15127–15145

- Lotero I, Trespalacios F, Grossmann IE, Papageorgiou DJ, Cheon MS. An MILP-MINLP decomposition method for the global optimization of a source based model of the multiperiod blending problem. *Comput Chem Eng*. 2016; 87: 13–35

- Castillo PAC, Castro PM, Mahalec V. Global optimization algorithm for large-scale refinery planning models with bilinear terms. *Ind Eng Chem Res*. 2017; 56(2): 530–548