Exploiting vector space properties for the global optimization of process networks

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Motivation

- The **optimization of process networks** is one of the most frequent problems that is addressed in **process systems engineering** (e.g. optimization of pooling networks, heat exchanger networks and water treatment networks)

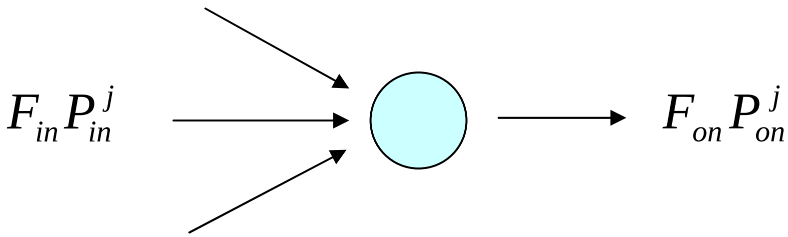
- **Mass and energy balances** are the common denominator of these systems and are often represented through equations with **bilinear terms**.

- Bilinearities lead to **nonconvex** problems hence, **global optimization** techniques are required.

- Variations of the **spatial branch and bound** framework are used to solve the problems. They heavily rely on **tight relaxations**.

Goal: Propose a methodology to find stronger relaxations for the global optimization of process networks.

Introduction



Building block of process networks

General mass and energy balance formulation

$$\sum_{i \in I_n} (F_{in} P_{in}^{j}) - F_{on} P_{in}^{j} = 0 \qquad \forall n \in N, \forall j \in J$$

$$\sum_{i \in I_n} F_{in} - F_{on} = 0 \qquad \forall n \in N$$

(MPB)

Sets:

N : Nodes in the network
I_n *: Streams entering node n and*
J : Property type

Vectorial Representation

For a given node *n* and property *j* we define the ***vectors***:

$$v_F = (F_1, F_2, ..., F_{|I|}, F_o) \quad v_E = (1,1,....,1,-1) \quad v_P = (P_1, P_2, ..., P_{|I|}, -P_o)$$

(MBP) can be represented as:

$$v_F . v_E = 0$$
$$v_P . v_E = 0$$

Or equivalently, in **vectorial form**:

3-Vector Representation

$$v_F \perp v_E$$
$$v_P \perp v_E$$

(VMPB)

The **interaction** between the vector spaces $\mathbf{v_F}$, $\mathbf{v_P}$ and the vector $\mathbf{v_E}$ is clearly **exposed** in the, 3-Vector Representation.

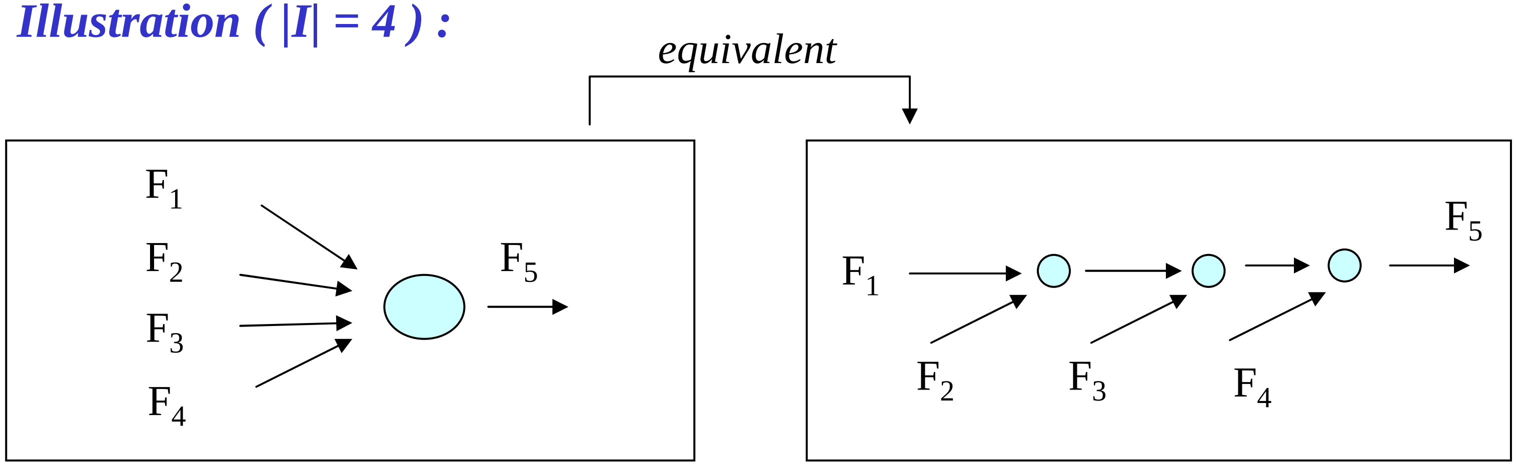
Minimal Set

We define a ***minimal set***, the set composed by three elements (i.e. |I|+1 = 3)

Lemma 1:

Any system of the form ***(VMBP)*** *can be decomposed as the* ***intersection*** *of |I|-1 3-Vector Representation of* ***minimal sets***

Illustration (|I| = 4) :



4 minimal sets

Properties of the minimal set

Lemma 2 : *The property vectors (v_P) and flow vectors (v_F) in a minimal set are related as follows:*

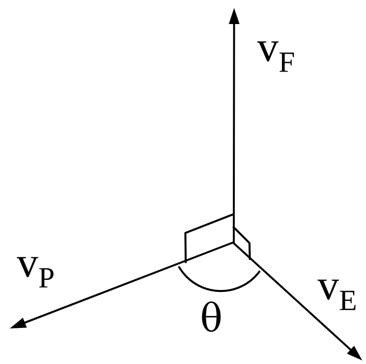
$$v_P \perp v_F \wedge v_F \perp v_E \Rightarrow v_P \times v_E \parallel v_F$$

Or equivalently

$$v_P . v_F = 0, v_E . v_F = 0 \Rightarrow v_P \times v_E = \alpha v_F$$

where $\alpha = \dfrac{\| v_P \| \sqrt{3} \sin\theta}{\| v_F \|}$, $0 \le \theta \le 2\pi$

Illustration:



The cross product between v_P and v_E is parallel to v_F

Properties of the minimal set (cont.)

Lemma 3: *The space defined by the minimal set is* ***nonconvex***

Illustration:

Given two points in the set

$$v^1_F = \{2,1,3\} \qquad v^2_F = \{1,1,2\}$$
$$v^1_P = \{1,1,-1\} \quad , \quad v^2_P = \{3,1,-2\} \qquad \in \quad \textbf{\textit{minimal set}}$$
$$v^1_E = \{1,1,-1\} \qquad v^2_E = \{1,1,-1\}$$

The following point, which is a convex combination, is not in the set

$$0.5v^1_F + 0.5v^2_F = v^{12}_F = \{1.5,1,2.5\}$$
$$0.5v^1_P + 0.5v^2_P = v^{12}_P = \{2,1,-1.5\} \qquad \notin \quad \textbf{\textit{minimal set}}$$
$$0.5v^1_E + 0.5v^2_E = v^{12}_E = \{1,1,-1\} \qquad v_F . v_P \neq 0$$

Convex relaxation of minimal set (Traditional Approach)

A ***traditional relaxation*** of (MPB) is given by replacing the bilinear terms with the ***McCormick*** convex envelopes.

$$\sum_{i\in\{1,2\}}(F_iP_i) - F_oP_o = 0$$

$$\sum_{i\in\{1,2\}}F_i - F_o = 0$$

$$FP_i \le F_iP_i^{up} + F_i^{lo}P_i - F_i^{lo}P_i^{up}$$

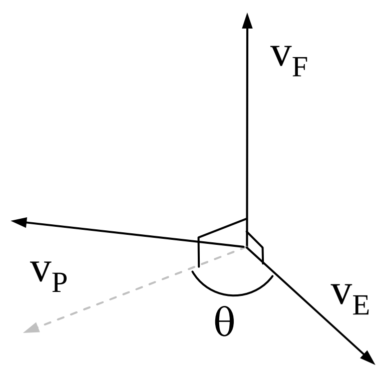
$$FP_i \le F_iP_i^{lo} + F_i^{up}P_i - F_i^{up}P_i^{lo}$$

$$FP_i \ge F_iP_i^{up} + F_i^{up}P_i - F_i^{up}P_i^{up}$$

$$v_F \times v_P = \alpha v_F$$

$$FP_i \ge F_iP_i^{lo} + F_i^{lo}P_i - F_i^{lo}P_i^{lo}$$

The orthoganality between v_P and v_F is lost!



$v_F \times v_P = \alpha v_F$ implicitly defines the orthogonality between v_P and v_F

Valid cuts from cross product

Based on ***Lemma 2*** the following is a valid cut

$$v_F \times v_P = \alpha v_F$$

Which in algebraic form reads

Nonconvex!

$$\begin{aligned} -P_2 + P_o &= \alpha F_1 \\ P_1 - P_o &= \alpha F_2 \\ P_1 - P_2 &= \alpha F_o \end{aligned} \qquad \textit{(CPC)}$$

From where the following ***linear cuts*** are derived:

$$\begin{aligned} \beta_i &\le \alpha F_i^{up} + \alpha^{lo} F_i - \alpha^{lo} F_i^{up} \\ \beta_i &\le \alpha F_i^{lo} + \alpha^{up} F_i - \alpha^{up} F_i^{lo} \\ \beta_i &\ge \alpha F_i^{up} + \alpha^{up} F_i - \alpha^{up} F_i^{up} \\ \beta_i &\ge \alpha F_i^{lo} + \alpha^{lo} F_i - \alpha^{lo} F_i^{lo} \end{aligned} \qquad i = o,1,2$$

where $\beta_1 = P_o - P_2$, $\beta_2 = P_1 - P_o$ and $\beta_o = P_1 - P_2$

Bounds for α

From the definition of ***cross product***:

$$\alpha^{up} = -\alpha^{lo} = \max\left(\frac{\| v_P \| \sqrt{3} \sin\theta}{\| v_F \|}\right) = \frac{\| v_P \|_{\max} \sqrt{3}}{\| v_F \|_{\min}} = \frac{\| {v_P}^{up} \| \sqrt{3}}{\| {v_F}^{lo} \|}$$

Tighter lower and upper bounds can be obtained by using ***(CPC)***:

$$\alpha^{up} = \min(\max\frac{-P_2 + P_o}{F_1}, \max\frac{-P_1 + P_o}{F_2}, \max\frac{P_2 - P_1}{F_o})$$

$$\alpha^{lo} = \max(\min\frac{-P_2 + P_o}{F_1}, \min\frac{P_1 - P_o}{F_2}, \min\frac{-P_2 + P_1}{F_o})$$

Proposed vs Traditional Approach

Proposition

*The proposed cuts are **not dominated by the McCormick** convex envelopes*

Illustration

Given the minimal set:

$$F_1P_1 + F_2P_2 = F_3P_3$$

$$F_1 + F_2 = F_3$$

where:

$$0.5 \le F_1 \le 2 \,,\ 1.5 \le F_2 \le 2.5,\ 2 \le F_3 \le 4.5$$

$$0.5 \le P_1 \le 1.5 \,,\ 0 \le P_2 \le 2,\ 0 \le P_3 \le 2$$

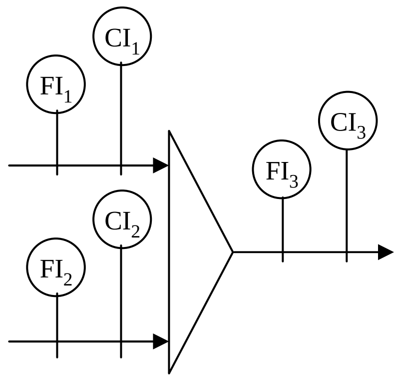
the region in the space with fixed F_1=0.5, F_2=2.3, F_3=2.8, P_1=1.2, P_2=0.1 is ***P_3 = [0.19-0.43]*** using the McCormcik envelopes and ***P_3 = [0.23-0.36]*** using the proposed cuts

Case Study
(Data Reconciliation)

Problem Statement:

Find the set of values of flows and composition that minimize the squared error when compared with the measurements.

System representation (Instance 1-2):



Formulation:

$$Min\ Z = w1(F_1 - FI_1)^2 + w2(F_2 - FI_2)^2 + w3(F_3 - FI_3)^2 + w4(F_4 - FI_4)^2 + w5(F_5 - FI_5)^2 + w6(F_6 - FI_6)^2$$

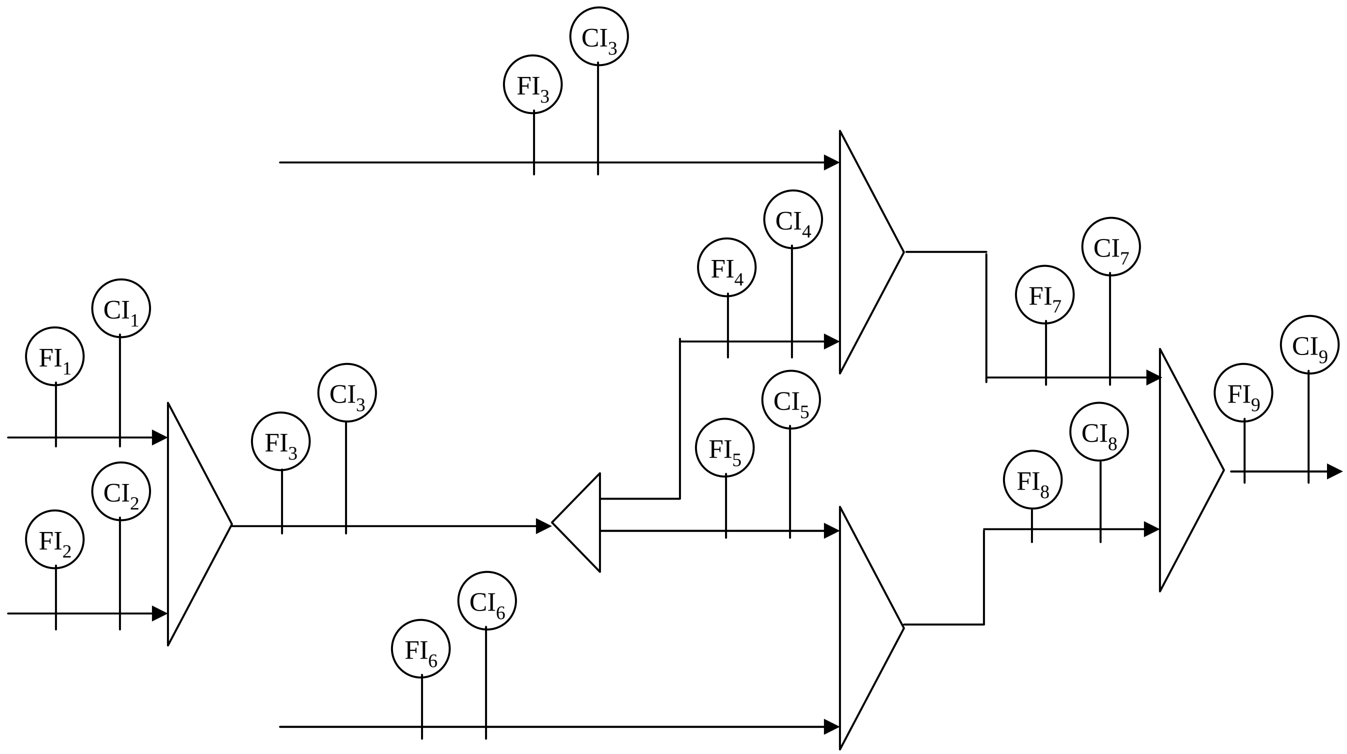
$$F_1 P_1 + F_2 P_2 = F_3 P_3$$
$$F_1 + F_2 = F_3$$

Nonconvex set

$$F_1^{lo} \le F_1 \le F_1^{up} \qquad F_2^{lo} \le F_2 \le F_2^{up}$$
$$P_1^{lo} \le P_1 \le P_1^{up} \qquad P_2^{lo} \le P_2 \le P_2^{up}$$

Numerical Results

System representation (Instance 3-4):



Numerical Results

		Traditional Approach			Proposed Approach		
Instance	GO	LB	Nodes	Time(s)	LB	Nodes	Time(s)
1	82.78	78.25	11	20	81.6	4	9
2	5.26	4.89	80	109	5.01	9	28
3	13.14	10.45	428	518	11.32	242	283
4	17.19	17.08	7	30	17.13	1	25

On average, the proposed approach led to **46%** improvement in lower bounds, **1/3 of nodes** necessary to find the solution and **1/2 the computational time**.

Conclusions

- Proposed a ***vectorial representation*** of the process network models.

- ***Exposed*** part of the ***interaction*** between the vector space defined by the ***flows and properties***.

- ***Proposed cuts*** that strengthen the relaxation given by traditional approaches.

- The ***performance of the method tested*** in several instances related to data reconciliation in process networks shows ***significant improvements***.