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# Piecewise Parametric Structure in the Pooling Problem – from Sparse Strongly-Polynomial Solutions to NP-Hardness

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**Abstract** The standard pooling problem is a NP-hard sub-class of non-convex quadratically-constrained optimization problems that commonly arises in process systems engineering applications. We take a parametric approach to uncovering topological structure and sparsity of the standard pooling problem in its  $p$ -formulation. The structure uncovered in this approach validates Professor Christodoulos A. Floudas' intuition that pooling problems are rooted in piecewise-defined functions. We introduce dominant active topologies to explicitly identify pooling problem sparsity and show that the sparse patterns of active topological structure are associated with a piecewise objective function. Finally, the paper explains the conditions under which sparsity vanishes and where the combinatorial complexity emerges to cross over the  $P/NP$  boundary. We formally present the results obtained and their derivations for various specialized pooling problem instances.

**Keywords** Standard pooling problem · Global optimization · Piecewise structure · Sparsity · Discretization ·  $P/NP$  boundary · Strongly-polynomial algorithms

## 1 Introduction

The standard pooling problem represents a NP-hard sub-class [3] of non-convex quadratically-constrained optimization problems with bilinear terms and may have a multiplicity of local minima [32]. Pooling problems model the computational difficulties associated with intermediate blending of heterogeneous feedstocks and therefore have direct application in process system engineering [33, 55]. Specific application domains include: petroleum refining [7, 19, 48], mining [13], wastewater treatment [34, 41], crude oil scheduling [38], natural gas production [49], etc. We recently showed that the standard pooling problems arises as a sub-problem pattern in general mixed-integer non-linear optimization (MINLP) [16].

Motivated by applications, Floudas and Visweswaran [21, 22, 56, 57] were the first to rigorously solve the pooling problem to global optimality. The Floudas and Visweswaran approach uses duality theory and Lagrangian relaxations. Subsequent global optimization contributions to solving the pooling problem include: making further Lagrangian relaxation contributions [1], developing alternative problem formulations [5, 10], augmenting models with reformulation-linearization cuts [41, 47, 50, 51] to create a provably dominant formulation [52], developing problem-specific polyhedral cuts based on small pooling networks [17, 18], and identifying the  $P/NP$  boundary with respect

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to the topological structure [3, 14, 30, 31]. More general techniques for non-convex quadratically-constrained optimization problems with bilinear terms are also appropriate for the pooling problem. The more general methods include: using convex envelopes to formulate a linear relaxation [2, 23, 40], developing a general branch-and-cut method [6], applying a sum-of-squares hierarchy [39], and using state-of-the-art global optimization MINLP solver software [9, 11, 12, 36, 44, 45, 52–54]. Further details are available in reviews discussing the pooling problem [5, 15, 29, 42].

But, despite significant attention to the pooling problem, deterministic global optimization algorithms can have significant optimality gaps and impractical or unknown convergence times on large-scale, industrially-relevant instances. These impractical convergence properties are interesting because Beale et al. [8] report that a simple, piecewise-linear program serves as a practical heuristic for small, pooling-like instances. Meyer and Floudas [41] had a similar intuition that very large pooling problems may be approached via piecewise-linear relaxation schemes. This intuition, which also appeared in Karuppiah and Grossmann [34], suggests that the pooling problem, a continuous nonlinear optimization problem (NLP), may be effectively approximated as a mixed-integer linear optimization problem (MILP). Further evidence for this intuition appears in several effective algorithms optimizing industrially-relevant pooling instances via piecewise-linear approaches, e.g. [25, 28, 35, 43, 46, 58]. Subsequent work used the standard pooling problem topology to develop a state-of-the-art MILP discretization heuristic with a performance bound [20, 26, 27].

This paper validates and substantiates Professor Floudas’ intuition by formalizing and characterizing the piecewise structures arising in standard pooling problem sub-instances. We build a bottom-up, intuitive understanding of the  $P/NP$  boundary of the single quality standard pooling problem by taking a parametric view and relaxing the flow availability box constraints. In the semantics of Boland et al. [14], e.g. Figure 1 of their manuscript, our approach unifies and generalizes the  $|K| = 1$  complexity results. Our parametric approach yields polynomial-time instances with a piecewise-linear or piecewise convex/concave monotone structure. We formalize these piecewise structures in standard pooling sub-instances that offer exact global solutions in polynomial time. The proofs lead to the unexpected outcome that the famous Haverly [32] pooling instances, i.e. the first-recorded pooling instances, are strongly-polynomial! The strongly-polynomial result for the Haverly [32] instances is remarkable because these case studies have been used as test cases for exponential algorithms for more than 35 years.

This manuscript also justifies the Beale et al. [8] observation that the linear approximation is most effective when only a few variables are active at once. Using patterns of dominating topologies, we explicitly identify pooling problem sparsity, i.e. a limited number of active flow variables. We show that these sparse patterns of active topological structure are associated with a piecewise objective function and we take advantage of these structures. Lastly, we explain the conditions under which such sparsity vanishes by reintroducing constraints on flow availability and, together with them, the combinatorial complexity needed to cross over the  $P/NP$ -time boundary.

The paper proceeds as follows: Section 2 introduces the standard pooling problem, notation and assumptions used throughout this paper; Section 3 analyzes the one pool, one output instance and uncovers both a piecewise-monotone structure and a strongly-polynomial time algorithm for solving it; Section 4 extends the results in Section 3 to instances with multiple outputs via additive decomposition over outputs; Section 5 extends Section 3 results to instances with multiple pools using problem sparsity; Section 6 discusses the implications and possible extensions of the results.

## 2 Standard pooling $p$ -formulation and assumptions used

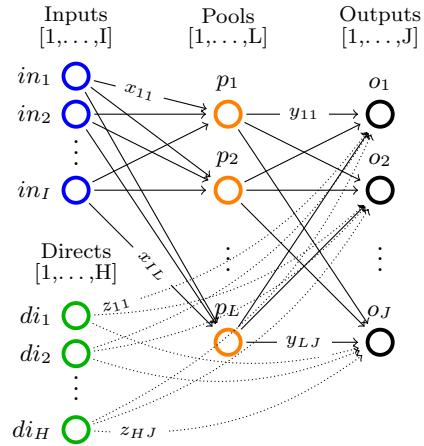
This manuscript unpacks standard pooling problem solutions by parametrizing with respect to pool concentrations. To effectively parameterize with respect to pool concentrations, this paper employs a concentration-based formulation, i.e. the  $p$ -formulation shown in Problem P–2.1 [5]. Table 1 introduces the notation used for indices, sets, variables, parameters, as well as for the

Table 1: Standard Pooling Problem Notation [42]

Type	Notation	Description
Indices	$i \in \{i \mid (i, \cdot) \in T_X \cup T_Z\}$	Input streams (raw materials or feed stocks)
	$l \in \overline{1, L}$	Pools (blending facilities)
	$j \in \overline{1, J}$	Output streams (end products)
	$k \in \overline{1, K}$	Attributes (qualities monitored)
Sets	$T_X$	$(i, l)$ pairs for which input to pool connection exists, $ T_X  = I$
	$T_Z$	$(i, j)$ pairs for which input to output connection exists, $ T_Z  = H$
	$T_Y$	$(l, j)$ pairs for which pool to output connection exists
Problem Type	$I + H - L - J - K$	$I + H$ feeds (inputs + directs), $L$ pools, $J$ outputs and $K$ qualities
	$I + H - L - J$	$I + H$ feeds (inputs + directs), $L$ pools, $J$ outputs and one quality
	$I - L - J$	(No directs) $I$ inputs, $L$ pools, $J$ outputs and one quality
	$H - L - J$	(No inputs) $H$ directs, $L$ pools, $J$ outputs and one quality
Variables	$x_{i,l}$	Flow from input $i$ to pool $l$
	$y_{l,j}$	Flow from intermediate pool node $l$ to output $j$
	$z_{i,j}$	Bypass flow directly from input feed stock $i$ to product $j$
	$p_{l,k}$	Level of quality attribute $k$ in pool $l$
Parameters	$f$	The objective function of the problem
	$\gamma_i$	Unit cost of raw material feed stock $i$
	$d_j$	Unit revenue for product $j$
	$A_i^L - A_i^U$	Availability bounds (required usage to max. availability) of input $i$
	$S_l$	Volumetric size capacity of pool $l$
	$D_j^L - D_j^U$	Demand bounds (required to limit demand) for product $j$
	$C_{i,k}$	Level of quality $k$ in raw material feed stock $i$
	$P_{j,k}^L - P_{j,k}^U$	Acceptable composition range of quality $k$ in product $j$

problem instance types analyzed in the following sections. Fig. 1 shows the topological structure of a standard pooling network, represented by a feed-forward flow network of 3 node layers.

Fig. 1: Standard pooling network. Note the feeds layer is separated into two groups of nodes: input nodes  $[1, \dots, I]$  that send flows to pools only and direct nodes  $[1, \dots, H]$  that send flows to outputs only. In general, one feed can send flows both to pools and outputs. In this case, any of feed's flows is assigned, based on the layer they are sent towards, to either an input or direct node corresponding to the feed. This explicit input/direct separation helps build a clear understanding of the problem sparsity/structure as related to flows to pools versus flows to outputs. The separation is generally adopted in the paper's figures, discussions or proofs, as needed.



Different flows pass between the three layers, having different concentrations of various qualities, e.g. crude oil chemical compositions. Input feeds  $in_1 - in_I$  send flows denoted by  $x$  variables to be linearly blended in  $L$  pools ( $p_1 - p_L$ ), that further distribute  $y$  flows to  $O$  outputs ( $o_1 - o_O$ ) to create blended products. Additionally,  $H$  direct feeds  $di_1 - di_H$  send  $z$  flows directly to the outputs layer. The standard pooling Problem P-2.1 consists of maximizing a profit function with profits and costs associated to each network flow, subject to flow constraints, e.g. feed availability, pool

capacity, output demands, flow balance at pools, and quality concentration constraints, e.g. quality balance at pools, product quality bounds at outputs. This manuscript addresses a somewhat more complex pooling problem than previous work analyzing the  $P/NP$  boundary [3, 14, 30, 31] by considering the direct feeds  $di_1 - di_H$ .

$$\begin{aligned}
& \text{(Objective)} \quad \max_{\substack{\{x_{i,l}\}, \{y_{l,j}\}, \\ \{z_{i,j}\}, \{p_{l,k}\}}} \sum_{(l,j) \in T_Y} d_j \cdot y_{l,j} + \sum_{(i,j) \in T_Z} d_j \cdot z_{i,j} - \sum_{(i,l) \in T_X} \gamma_i \cdot x_{i,l} - \sum_{(i,j) \in T_Z} \gamma_i \cdot z_{i,j} \\
& \text{(Feed Availability)} \quad \left[ A_i^L \leq \sum_{l:(i,l) \in T_X} x_{i,l} + \sum_{j:(i,j) \in T_Z} z_{i,j} \leq A_i^U \quad \forall i \right. \\
& \text{(Pool Capacity)} \quad \left[ \sum_{i:(i,l) \in T_X} x_{i,l} \leq S_l \quad \forall l \right. \\
& \text{(Product Demand)} \quad \left[ D_j^L \leq \sum_{l:(l,j) \in T_Y} y_{l,j} + \sum_{i:(i,j) \in T_Z} z_{i,j} \leq D_j^U \quad \forall j \right. \\
& \text{(Material Balance)} \quad \left[ \sum_{i:(i,l) \in T_X} x_{i,l} - \sum_{j:(l,j) \in T_Y} y_{l,j} = 0 \quad \forall l \right. \\
& \text{(Product Quality)} \quad \left[ \begin{aligned} & \sum_{l:(l,j) \in T_Y} p_{l,k} \cdot y_{l,j} \geq P_{j,k}^L \left( \sum_{l:(l,j) \in T_Y} y_{l,j} + \sum_{i:(i,j) \in T_Z} z_{i,j} \right) \\ & + \sum_{i:(i,j) \in T_Z} C_{i,k} \cdot z_{i,j} \leq P_{j,k}^U \left( \sum_{l:(l,j) \in T_Y} y_{l,j} + \sum_{i:(i,j) \in T_Z} z_{i,j} \right) \end{aligned} \right. \quad \forall j, k \\
& \text{(Quality Balance)} \quad \left[ \sum_{i:(i,l) \in T_X} C_{i,k} x_{i,l} = p_{l,k} \sum_{j:(l,j) \in T_Y} y_{l,j} \quad \forall l, k \right. \\
& \text{(Hard Bounds)} \quad \left[ \begin{aligned} & 0 \leq x_{i,l} \leq \min \left\{ A_i^U, \sum_{j:(l,j) \in T_Y} D_j^U, S_l \right\} \quad \forall (i,l) \in T_X \\ & 0 \leq y_{l,j} \leq \min \left\{ \sum_{i:(i,l) \in T_X} A_i^U, D_j^U, S_l \right\} \quad \forall (l,j) \in T_Y \\ & 0 \leq z_{i,j} \leq \min \left\{ A_i^U, D_j^U \right\} \quad \forall (i,j) \in T_Z \\ & \min_i C_{i,k} \leq p_{l,k} \leq \max_i C_{i,k} \quad \forall l, k \end{aligned} \right.
\end{aligned} \tag{P-2.1}$$

**Remark 2.1** In Problem P-2.1, the upper hard bounds on variable sets  $\{x\}$ ,  $\{y\}$ ,  $\{z\}$  are redundant and can be dropped. These upper hard bounds are implicitly met by simultaneously enforcing the constraints on feed availability, pool capacity, product demand and material balance. Similarly, the hard bounds on  $p_{l,k} \forall l, k$  can be dropped, as they are implicitly met by replacing all  $y$  variables in the quality balance with  $x$  variables from the material balance.

**Assumption 2.2** Problem P-2.1 is restricted to a single quality and assumed feasible, with dropped constraints on feed availability and pool capacity and fixed product demands  $D_j > 0, \forall j$ .

Based on Remark 2.1 and Assumption 2.2, after dropping indices  $k$  for simplicity and denoting the objective function with  $f$ , Problem P-2.1 becomes:

$$\begin{aligned}
 & \max_{\{x_{i,l}\}, \{y_{l,j}\}, \{z_{i,j}\}, \{p_l\}} f \\
 f = & \sum_{(l,j) \in T_Y} d_j \cdot y_{l,j} + \sum_{(i,j) \in T_Z} d_j \cdot z_{i,j} - \sum_{(i,l) \in T_X} \gamma_i \cdot x_{i,l} - \sum_{(i,j) \in T_Z} \gamma_i \cdot z_{i,j} \\
 \text{s.t.} & \sum_{l:(l,j) \in T_Y} y_{l,j} + \sum_{i:(i,j) \in T_Z} z_{i,j} = D_j \quad \forall j \\
 & \sum_{i:(i,l) \in T_X} x_{i,l} - \sum_{j:(l,j) \in T_Y} y_{l,j} = 0 \quad \forall l \\
 & P_j^L D_j \leq \sum_{l:(l,j) \in T_Y} p_l \cdot y_{l,j} + \sum_{i:(i,j) \in T_Z} C_i \cdot z_{i,j} \leq P_j^U D_j \quad \forall j \\
 & \sum_{i:(i,l) \in T_X} C_i x_{i,l} = p_l \sum_{j:(l,j) \in T_Y} y_{l,j} \quad \forall l \\
 & 0 \leq x_{i,l} \quad \forall (i,l) \in T_X, \quad 0 \leq y_{l,j} \quad \forall (l,j) \in T_Y, \quad 0 \leq z_{i,j} \quad \forall (i,j) \in T_Z.
 \end{aligned} \tag{P-2.2}$$

The next sections analyze bottom-up instances of Problem P-2.2 based on topological restrictions and prove strongly-polynomial time complexity for several topologies. Our analysis maps topological restrictions and Assumption 2.2 to sparse structures determining the contour of the P/NP-hard boundary for Problem P-2.2 instances.

### 3 Instance I+H-1-1: One Pool, One Output

This section analyzes the topological restriction of Problem P-2.2 with  $I + H$  feeds ( $I$  inputs,  $H$  directs), one pool, and one output. For simplicity of notation, single indices  $l$  and  $j$  are dropped from variables and parameters via the notation transformations  $T_Z \leftarrow \{i : (i,j) \in T_Z\}$ ,  $T_X \leftarrow \{i : (i,l) \in T_X\}$  leading to the restricted Problem P-3.3.

$$\begin{aligned}
 & \max_{\{x_i\}, y, \{z_i\}, p} f \\
 f = & d \cdot y + \sum_{i \in T_Z} d \cdot z_i - \sum_{i \in T_X} \gamma_i \cdot x_i - \sum_{i \in T_Z} \gamma_i \cdot z_i \\
 \text{s.t.} & y + \sum_{i \in T_Z} z_i = D \\
 & \sum_{i \in T_X} x_i - y = 0 \\
 & P^L D \leq p \cdot y + \sum_{i \in T_Z} C_i \cdot z_i \leq P^U D \\
 & \sum_{i \in T_X} C_i x_i = p \cdot y \\
 & 0 \leq x_i \quad \forall i \in T_X, \quad 0 \leq y, \quad 0 \leq z_i \quad \forall i \in T_Z
 \end{aligned} \tag{P-3.3}$$

$$\begin{aligned}
 & \max_{\{x_i\}, \{z_i\}, p} f = \max_p (f^*(p)) \\
 f^*(p) = & \max_{\{x_i\}, \{z_i\}} f(p) \\
 f(p) = & d \cdot D - \sum_{i \in T_X} \gamma_i \cdot x_i - \sum_{i \in T_Z} \gamma_i \cdot z_i \\
 \text{s.t.} & \sum_{i \in T_X} x_i + \sum_{i \in T_Z} z_i = D \\
 & P^L \leq \left( \sum_{i \in T_X} C_i x_i + \sum_{i \in T_Z} C_i z_i \right) / D \leq P^U \\
 & \sum_{i \in T_X} C_i x_i = p \cdot \sum_{i \in T_X} x_i \\
 & 0 \leq x_i \quad \forall i \in T_X, \quad 0 \leq z_i \quad \forall i \in T_Z
 \end{aligned} \tag{P-3.4}$$

Variables  $p, y$  can be eliminated from Problem P-3.3 by directly substituting all  $y, p \cdot y$  terms from

their constraints. Thus,  $f$  can be rewritten:

$$\begin{aligned} f &= d \cdot y + \sum_{i \in T_Z} d \cdot z_i - \sum_{i \in T_X} \gamma_i \cdot x_i - \sum_{i \in T_Z} \gamma_i \cdot z_i = \sum_{i \in T_X} (d - \gamma_i) \cdot x_i + \sum_{i \in T_Z} (d - \gamma_i) \cdot z_i \\ &= d \cdot D - \sum_{i \in T_X} \gamma_i \cdot x_i - \sum_{i \in T_Z} \gamma_i \cdot z_i. \end{aligned}$$

In Problem P–3.4, we eliminate  $y$  but retain  $p$  as a parameter controlling flows  $x_i$ ,  $\forall i \in T_X$  relative to each other. Also eliminating  $p$  from Problem P–3.3 produces an easily-solvable linear program (LP), but the LP solution is a black-box. Retaining parameter  $p$  allows us to analytically understand the optimal solutions for Problem P–3.4, together with any problem structure. In particular, the  $p$ -parametric form of the Problem P–3.4 objective may be used to break the  $p$ -interval  $[\min_i C_i, \max_i C_i]$  into sub-intervals where special properties of  $f$  arise. Section 4 uses this parametric approach for solving non-convex/non-linear instances in strongly-polynomial time.

Active sets, dominance relations and breakpoints are essential building blocks to find the structure of  $f^*(p)$  in Problem P–3.4 and are all introduced in Definitions 3.1–3.4.

**Definition 3.1** (*Active sets, objective function and cost function*)

Set  $A$  of nodes from the feed layer is:

- An **input active set** if  $A \subseteq T_X$ ,  $x_i > 0 \forall i \in A$ ,  $x_i = 0 \forall i \in T_X \setminus A$ ,  $z_i = 0 \forall i \in T_Z$ .
- A **direct active set** if  $A \subseteq T_Z$ ,  $z_i > 0 \forall i \in A$ ,  $z_i = 0 \forall i \in T_Z \setminus A$ ,  $x_i = 0 \forall i \in T_X$ .
- A **mixed active set** if  $A \subseteq T_X \cup T_Z$ ,  $x_i > 0 \forall i \in A \cap T_X \neq \emptyset$ ,  $z_i > 0 \forall i \in A \cap T_Z \neq \emptyset$ ,  $z_i = 0 \forall i \in T_Z \setminus A$ ,  $x_i = 0 \forall i \in T_X \setminus A$ .

For an active set  $A$  in Problem P–3.4, the objective function  $f$  is given by,

$$f = \begin{cases} f_A(p) = d \cdot D - \sum_{i \in A \cap T_X} \gamma_i x_i - \sum_{i \in A \cap T_Z} \gamma_i z_i, & \text{if } A \text{ is an input or mixed active set,} \\ f_A = d \cdot D - \sum_{i \in A} \gamma_i z_i, & \text{if } A \text{ is a direct active set,} \end{cases} \quad (1)$$

where  $f$  is not  $p$ -parametric in the second case of no input flow to the pool since pool concentration  $p$  is undefined. Let  $h = d \cdot D - f$  denote the cost function associated with objective function  $f$ .

**Definition 3.2** (*Feasibility with respect to product quality constraints*)

A Problem P–3.4 active set is **feasible** if the product quality bounds  $[P^L, P^U]$  are met, i.e. the second constraint holds. An infeasible active set is not a valid Problem P–3.4 solution and is therefore strictly dominated by any feasible active set (see Definition 3.3).

**Definition 3.3** (*Dominance and breakpoints between active sets*)

Let  $A_1, A_2$  be feasible input/mixed active sets. Let  $f_A^*(p)$  be the optimal solution to Problem P–3.4 and  $h_A^*(p)$  its corresponding optimal cost, assuming active set  $A$  and fixed  $p$ .

- Set  $A_1$  **dominates**  $A_2$  **at**  $p$  (in the sense of maximized objective function profitability) when,

$$\mathbf{A}_1 \succeq_p \mathbf{A}_2 \Leftrightarrow f_{A_1}^*(p) \geq f_{A_2}^*(p) \Leftrightarrow h_{A_1}^*(p) \leq h_{A_2}^*(p). \quad (2)$$

- Pool concentration  $p$  is a **breakpoint between**  $A_1$  **and**  $A_2$  if:

$$\mathbf{A}_1 \asymp_p \mathbf{A}_2 \Leftrightarrow f_{A_1}^*(p) = f_{A_2}^*(p) \Leftrightarrow h_{A_1}^*(p) = h_{A_2}^*(p). \quad (3)$$

- The dominance relation also extends to direct active sets, but in this case  $f$  is not parametric on  $p$ . Consequently, when comparing two direct active sets, dominance is established similarly via Eq. (2) but independent of  $p$ , and as such no breakpoints exist. Thus, for fixed  $p$ , a total order can be established over the set of all possible active sets.

**Definition 3.4** (*Dominant active sets and dominance breakpoints*)

Let  $\mathcal{A}^*(p)$  be the **dominant active set** (overall) at  $p$  if

$$\mathcal{A}^*(p) = \arg \max_{\{\mathcal{A}_I, \mathcal{A}_D, \mathcal{A}_M\}} (f_{\mathcal{A}_I}^*(p), f_{\mathcal{A}_D}^*, f_{\mathcal{A}_M}^*(p)) = \arg \min_{\{\mathcal{A}_I, \mathcal{A}_D, \mathcal{A}_M\}} (h_{\mathcal{A}_I}^*(p), h_{\mathcal{A}_D}^*, h_{\mathcal{A}_M}^*(p)) \quad (4)$$

and the optimal objective solution of Problem P–3.4 is  $f^* = \max_p f_{\mathcal{A}^*(p)}^*(p)$ , where:

- $\mathcal{A}_I$  is the **dominant input active set** at  $p$  if  $\mathcal{A}_I(p) = \arg \max_{A \subseteq T_X} f_A^*(p)$ .
- $\mathcal{A}_M$  is the **dominant mixed active set** at  $p$  if  $\mathcal{A}_M(p) = \arg \max_{A \subseteq T_X \cup T_Z, A \cap T_X \neq \emptyset, A \cap T_Z \neq \emptyset} f_A^*(p)$ .
- $\mathcal{A}_D$  is the **dominant direct active set** if  $\mathcal{A}_D = \arg \max_{A \subseteq T_Z} f_A^*$ .

A **dominance breakpoint** represents a  $p$  value where the dominant active set changes, i.e.:

$$\forall \epsilon > 0 \mathcal{A}^*(p - \epsilon) = A_1 \neq A_2 = \mathcal{A}^*(p + \epsilon) \text{ and } A_1 \succ_p A_2. \quad (5)$$

**Input and mixed dominance breakpoints** are similarly defined as in Eq. (5) but with  $\mathcal{A}^*$  replaced by  $\mathcal{A}_I$  and  $\mathcal{A}_M$ , respectively. Let the sets of input and mixed dominance breakpoints be denoted by  $\mathcal{B}_I$  and  $\mathcal{B}_M$ , respectively.

The input, direct and mixed active sets have different dominance properties and thus the analysis proceeds in Sections 3.1–3.3 by active set type. Section 3.1 ignores directs and product quality constraints and focuses only on inputs. Since directs are ignored, the pool concentration  $p$  represents the output concentration, and hence  $p$  is assumed free of product quality bounds. The analysis of the  $p$ -parametric optimal objective  $f^*(p)$  reveals a piecewise-linear structure associated with pairs of inputs acting as the dominant input active set. Section 3.2 treats the complementary case, ignoring inputs and focusing only on directs while assuming product quality constraints. Since inputs and therefore the pool are assumed to send no flow in this case, the optimal objective  $f^*$  and dominant direct active set are found independently of  $p$ . Finally, Section 3.3 integrates the Sections 3.1–3.2 results, combining both inputs and directs under assumed product quality constraints to reveal a sparse, piecewise-monotone structure of the  $p$ -parametric optimal objective  $f^*(p)$ .

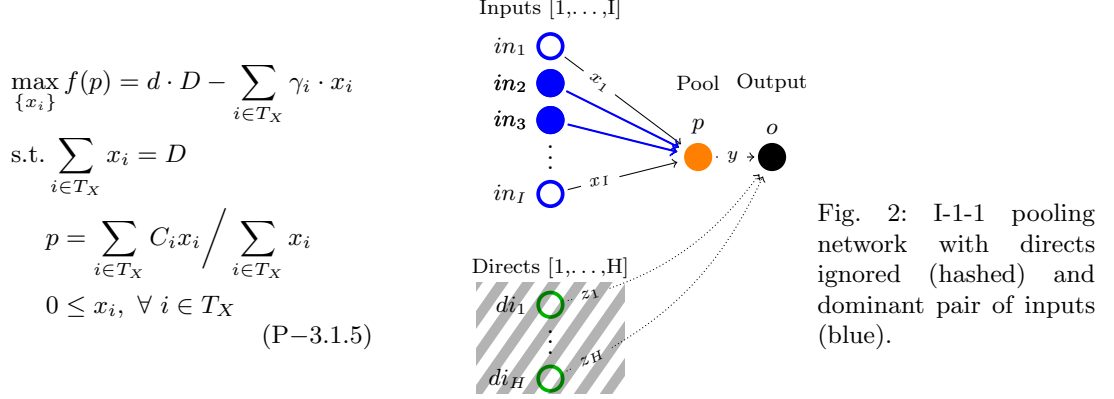
Sections 3.1–3.3 analytically and parametrically identifies all (dominance) breakpoints, sparse dominant active sets and associated  $p$ -parametric solutions for Problem P–3.4. This analysis leads to a strongly-polynomial algorithm in Section 3.3 for solving the I+H-1-1 instance formalized in Problem P–3.4. Furthermore the full structure of the  $p$ -parametric optimal objective function  $f^*(p)$  developed in Section 3.3 is vital for Sections 4–5.

**Remark 3.5** For any  $i, j \in T_X \cup T_Z$  with  $i \neq j$ ,  $C_i = C_j$ , if  $\gamma_i \leq \gamma_j$  precedence is given to the node  $i$  with cheaper flow, or at cost equality a random choice is made. After pre-filtering all feeds of equal concentrations on cost criteria, we are assured  $\forall i, j \in T_X \cup T_Z, i \neq j$  that  $C_i \neq C_j$ . For any  $i, j \in T_X \cup T_Z$  with  $i \neq j$ ,  $C_i < C_j$  if  $\gamma_i = \gamma_j$  precedence is given to  $i$  if  $C_i \in [P^L, P^U]$ ,  $C_j \notin [P^L, P^U]$  and vice versa. We apply the enumerated precedence rules throughout Section 3. This pre-filtering avoids undefined expressions, e.g. denominators with value zero in the subsequent sections.

### 3.1 Inputs-Only Analysis (I-1-1 Sub-Case)

This subsection considers the Problem P–3.4 restriction with no direct flows to the output ( $z_i = 0, \forall i \in T_Z$ ) and no product quality constraints on the pool concentration  $p$ . The resulting Problem P–3.1.5 is  $p$ -parametric, and thus we seek to find both the optimal solution and the full  $p$ -parametric structure. A dominance ordering is built bottom-up through increasing cardinalities of active sets via Proposition 3.1.3, Corollary 3.1.4, and Lemmas 3.1.5–3.1.6. Corollary 3.1.7 concludes the ordering, finding the dominant input active set at  $p$ ,  $\mathcal{A}_I(p)$ . Theorem 3.1.8 then finds all

input dominance breakpoints  $\mathcal{B}_I$  and the optimal solution. More importantly, Theorem 3.1.8 also identifies the full piecewise-linear structure of the  $p$ -parametric optimal objective  $f^*(p)$  motivated by Lemma 3.1.1. The piecewise structure is expanded in Section 3.3 in the presence of directs and product quality constraints, but remains fundamental to all analytical solutions found in the paper, including Sections 4–5.





**Corollary 3.1.4** If  $i, j, k \in T_X$ , then:

$$ij = \{i, j\} \succeq_p kj = \{k, j\} \Leftrightarrow \frac{(C_j - p)(C_k(\gamma_j - \gamma_i) + C_i(\gamma_k - \gamma_j) + C_j(\gamma_i - \gamma_k))}{(C_i - C_j)(C_k - C_j)} < 0. \quad (10)$$

*Proof* Follows directly from Eq. (9a) by replacing  $l$  with  $j$ . Because  $p$  is a linear combination of both  $C_i, C_j$  and  $C_k, C_j$ , Eq. (10) implies  $C_i, C_k > p > C_j$  or  $C_j > p > C_i, C_k$ . Thus, Eq. (10) is invariant to whether  $C_j > p$  or  $C_j < p$ , as expected. Also, Eq. (10) changes sign when permuting  $i$  and  $k$  (or the compared pairs) but is invariant under a permutation of  $i$  and  $j$ .  $\square$

**Lemma 3.1.5** If  $i, j \in T_X$ , then  $\forall k \in T_X$ ,  $\{i, j\} \succeq_p \{i, k\}$  or  $\{i, j\} \succeq_p \{k, j\} \Rightarrow \{i, j\} \succeq_p \{i, j, k\}$ .

*Proof* Let  $P = \{i, j\}$ ,  $T = \{i, j, k\}$ . According to Eq. (2), the optimal costs (optimality \* superscript omitted for simplicity) for  $P, T$  are:

$$\left\{ \begin{array}{l} h_P(p) = \gamma_i x_i + \gamma_j x_j, \quad \text{with } p = \frac{C_i x_i + C_j x_j}{x_i + x_j}, \quad D = x_i + x_j, \\ h_T(p) = \gamma_i x'_i + \gamma_j x'_j + \gamma_k x'_k, \quad \text{with } p = \frac{C_i x'_i + C_j x'_j + C_k x'_k}{x'_i + x'_j + x'_k}, \quad D = x'_i + x'_j + x'_k. \end{array} \right.$$

Substituting  $x_i, x_j$  from Eq. (7) results in  $h_P(p) = \frac{D(\gamma_i(p - C_j) - \gamma_j(p - C_i))}{C_i - C_j}$ . Solving similarly for  $x'_i, x'_j$  in terms of  $x'_k$ , from pool concentration and flow demand, it follows that:

$$x'_i = \frac{D(p - C_j) - x'_k(C_k - C_j)}{C_i - C_j}, \quad x'_j = \frac{-D(p - C_i) + x'_k(C_k - C_i)}{C_i - C_j}.$$

Introducing the above  $x'_i, x'_j$  formulas into  $h_T(p)$  and subtracting  $h_P(p)$  results in:

$$\begin{aligned} h_T(p) - h_P(p) &= \gamma_k x'_k + x'_k \left( \gamma_j \frac{C_k - C_i}{C_i - C_j} - \gamma_i \frac{C_k - C_j}{C_i - C_j} \right) \\ &= x'_k \frac{C_k(\gamma_j - \gamma_i) + C_i(\gamma_k - \gamma_j) + C_j(\gamma_i - \gamma_k)}{C_i - C_j}. \end{aligned} \quad (11)$$

Therefore,  $P \succeq_p T \Leftrightarrow h_P(p) \leq h_T(p) \Leftrightarrow x'_k \frac{C_k(\gamma_j - \gamma_i) + C_i(\gamma_k - \gamma_j) + C_j(\gamma_i - \gamma_k)}{C_i - C_j} \leq 0 \Leftrightarrow$  RHS condition in Eq. (10). The last equivalence follows because the denominator of Eq. (10) and  $x'_k$  are positive,  $C_j - p$  and  $C_j - C_i$  have same sign ( $C_j < p < C_i$  or  $C_j > p > C_i$ ), and the remaining factor is identical. This equivalence and the invariance of Eq. (10) to permuting  $i, j$  concludes the proof.  $\square$

**Lemma 3.1.6** For fixed  $p$ , if input active pair  $\{i, j\}$  dominates at  $p$  all other input pairs then:

- (i)  $\{i, j\}$  dominates at  $p$  any triple  $\{k, l, m\}$  for any  $k, l, m \in T_X$ .
- (ii)  $\{i, j\}$  dominates at  $p$  any input active set of any higher cardinality.

*Proof* (i) Let  $P = \{i, j\}$ ,  $T = \{k, l, m\}$ . From Lemma 3.1.5, if  $P_T \succeq_p P$  for  $P_T \subset T$ ,  $\forall P \subset T, P \neq P_T$ , then  $P_T \succeq_p T$ . Since  $P$  dominates any other pair including  $P_T$ , by transitivity  $P \succeq_p T$ .

(ii) The proof focuses on showing first that,

$$\left. \begin{array}{l} \forall S \subseteq T_X, S = \{s_1, \dots, s_n\}, 2 < |S| = n \leq |T_X| = I, \\ \text{assuming } P_S = \{s_1, s_2\} = \arg \min_{\{s_i, s_j\} \subseteq S} \frac{\gamma_{s_i}(p - C_{s_j}) + \gamma_{s_j}(C_{s_i} - p)}{C_{s_i} - C_{s_j}} \end{array} \right\} \Rightarrow P_S \succeq_p S. \quad (12)$$

Consider a suitable choice of  $S$  and its corresponding pair subset  $P_S$  that dominates at  $p$  any alternative pair subsets of  $S$ . To prove  $P_S \succeq_p S$ , following Eq. (2), consider the optimal costs (omitted \* superscript) for both  $P_S$  and  $S$  with:

$$h_{P_S}(p) = \gamma_{s_1}x_{s_1} + \gamma_{s_2}x_{s_2}, \quad h_S(p) = \sum_{i=1}^n \gamma_{s_i}x'_{s_i}, \quad D = x_{s_1} + x_{s_2} = \sum_{i=1}^n x'_{s_i} \quad (13)$$

Consider the weights  $w_{s_i} = x'_{s_i} / (D - x'_{s_1} - x'_{s_2}) \quad \forall i \in \overline{3, n}$ , which, due to Eq. (13), sum up to 1 and  $w_{s_i} \in [0, 1]$ . Consequently,

$$\begin{aligned} h_{P_S}(p) &= \sum_{i=3}^n (\gamma_{s_1}x_{s_1} + \gamma_{s_2}x_{s_2})w_{s_i} &&= \sum_{i=3}^n \underbrace{((w_{s_i}\gamma_{s_1})x_{s_1} + (w_{s_i}\gamma_{s_2})x_{s_2})}_{h_{P_S}^i(p)} \\ h_S(p) &= \sum_{i=3}^n (\gamma_{s_1}x'_{s_1} + \gamma_{s_2}x'_{s_2})w_{s_i} + \gamma_{s_i}x'_{s_i} &&= \sum_{i=3}^n \underbrace{((w_{s_i}\gamma_{s_1})x'_{s_1} + (w_{s_i}\gamma_{s_2})x'_{s_2} + \gamma_{s_i}x'_{s_i})}_{h_S^i(p)}, \end{aligned} \quad (14)$$

where in the last summation expressions for  $h_{P_S}$  and  $h_S$  the weights are viewed to act only on the costs  $\gamma_{s_1}, \gamma_{s_2}$  of the nodes in pair  $P_S$ . For any arbitrary  $i \in \overline{3, n}$ , with  $T_i = \{s_1, s_2, s_i\}$ , we have

$$\begin{aligned} h_{P_S}^i(p) - h_S^i(p) &\stackrel{\text{Eq. (11)}}{=} x'_{s_i} \frac{C_{s_i}(w_{s_i}\gamma_{s_2} - w_{s_i}\gamma_{s_1}) + C_{s_1}(\gamma_{s_i} - w_{s_i}\gamma_{s_2}) + C_{s_2}(w_{s_i}\gamma_{s_1} - \gamma_{s_i})}{C_{s_2} - C_{s_1}} \\ &= w_{s_i}x'_{s_i} \left( \frac{C_{s_i}(\gamma_{s_2} - \gamma_{s_1}) + C_{s_2}\gamma_{s_1} - C_{s_1}\gamma_{s_2} - \gamma_{s_i}}{C_{s_2} - C_{s_1}} - \frac{1}{w_{s_i}} \right) \\ &< w_{s_i}x'_{s_i} \left( \frac{C_{s_i}(\gamma_{s_2} - \gamma_{s_1}) + C_{s_2}\gamma_{s_1} - C_{s_1}\gamma_{s_2}}{C_{s_2} - C_{s_1}} - \gamma_{s_i} \right) \\ &= w_{s_i}x'_{s_i} \frac{C_{s_i}(\gamma_{s_2} - \gamma_{s_1}) + C_{s_1}(\gamma_{s_i} - \gamma_{s_2}) + C_{s_2}(\gamma_{s_1} - \gamma_{s_i})}{C_{s_2} - C_{s_1}} \\ &\stackrel{\text{Eq. (11)}}{\Rightarrow} h_{P_S}^i(p) \leq h_S^i(p) \Leftrightarrow h_{P_S}(p) \leq h_S(p) \Leftrightarrow P_S \succeq_p T_i. \end{aligned} \quad (15)$$

Since Eq. (12) assumes  $P_S \succeq_p \{s_1, s_i\} \quad \forall i \in \overline{3, n}$ , Lemma 3.1.5 implies  $P_S \succeq_p T_i \quad \forall i \in \overline{3, n}$ , so

$$h_{P_S}^i(p) \leq h_S^i(p) \quad \forall i \in \overline{3, n} \Rightarrow \sum_{i=3}^n h_{P_S}^i(p) \leq \sum_{i=3}^n h_S^i(p) \Rightarrow h_{P_S}(p) \leq h_S(p) \Rightarrow P_S \succeq_p S. \quad (16)$$

Thus, by transitivity, for any subset  $S$  of  $T_X$  as in Eq. (12),  $P \succeq_p P_S \succeq_p S$ , concluding the proof.  $\square$

**Corollary 3.1.7** (*Dominant input active set at  $p$* )

For fixed  $p$ , if an input active pair  $ij = \{i, j\}$  dominates at  $p$  any alternative pair, i.e.:

$$ij = \arg \min_{\{k, l\} \subseteq T_X} \gamma_{kl}(p) = \arg \min_{\{k, l\} \subseteq T_X} \frac{\gamma_k(p - C_l) + \gamma_l(C_k - p)}{C_k - C_l}, \quad (17)$$

then  $\mathcal{A}_I(p) = ij$  for Problem P-3.1.5 (follows directly from Proposition 3.1.3 and Lemma 3.1.6).

**Theorem 3.1.8** (*Inputs-only optimal solution and input dominance breakpoints*)

(i) Input dominance breakpoints can occur only at input concentrations  $C_i$ ,  $i \in T_X$ , hence,

$$f^* = \max_{i \in T_X} f^*(C_i) = \max_{i \in T_X} D(d - \gamma_i),$$

which requires  $I$  (number of inputs) evaluations.

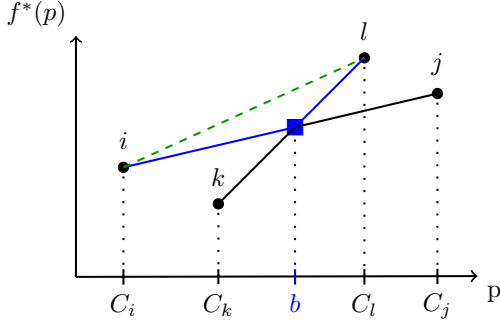


Fig. 3:  $i-j$  and  $l-k$  lines represent  $f^*(p)$  between individual node concentrations for pairs  $\{i, j\}$  and  $\{l, k\}$ , respectively -  $b$  is the breakpoint concentration between the two node pairs. The bold blue lines show the optimal objective if  $b$  is a dominance breakpoint, and the green dashed line shows the optimal objective otherwise.

- (ii) A full description of  $f^*(p)$  can be obtained in strongly-polynomial time  $O(I^3)$ , with the set  $\mathcal{B}_I$  of input dominance breakpoints,

$$\mathcal{B}_I = \left\{ C_i \mid i \in T_X, \gamma_i < \arg \min_{\{k,l\} \subseteq T_X \setminus \{i\}} \gamma_{kl}(C_i) \right\}. \quad (18a)$$

Between any two consecutive elements of  $\mathcal{B}_I$ , the dominant input active set remains constant, i.e.

$$C_i, C_j \in \mathcal{B}_I, \mathcal{B}_I \cap (C_i, C_j) = \emptyset \Rightarrow \mathcal{A}_I(p) = \{i, j\} \quad \forall p \in (C_i, C_j) \quad (18b)$$

*Proof* (i) Since Corollary 3.1.7 implies  $|\mathcal{A}_I(p)| = 2$ , let two such dominant active input pairs,  $\{i, j\}$  and  $\{k, l\}$ , and w.l.o.g. assume  $C_i < C_j, C_k < C_l$ . Assume, to achieve a contradiction, that an input dominance breakpoint occurs at  $b$ , where  $b \in (C_i, C_j) \cap (C_k, C_l)$ . Consequently, again w.l.o.g. assume  $\{k, l\} \succeq_p \{i, j\} \forall p \in (b, C_l)$ . As a result, in the geometric construction of Fig. 3,  $i-l-j-k$  forms a quadrilateral with  $f^*(b)$  at the intersection of its diagonals. Notice,  $\forall p \in (C_i, C_l)$ , the  $f_{\{i,l\}}^*(p)$  values obtained on the side  $i-l$  (dashed green) are higher than the optimal objective values obtained by going through the breakpoint  $b$  (lines in bold blue), contradiction. Therefore no input dominance breakpoint can occur at a pool concentration  $b \notin \{C_i \mid i \in T_X\}$ . Since Lemma 3.1.1 implies  $f^*(p)$  is linear between any two input dominance breakpoints when an input pair is active, the assertion made follows.

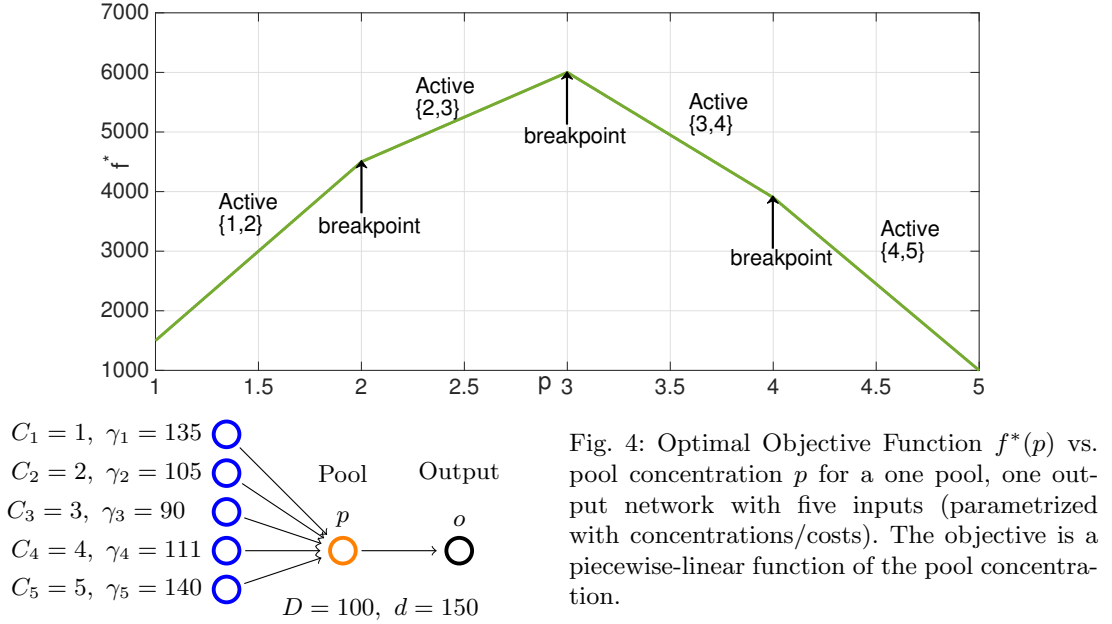
(ii) To fully describe  $f^*(p)$ , if  $C_i$  for fixed  $i \in T_X$  is an input dominance breakpoint, then, according to Eq. (17), node  $i$  must strictly dominate at  $C_i$  any input pair not containing it. Eq. (18b) follows via the definitions of  $\mathcal{B}_I, \mathcal{A}_I$ .  $\square$

**Remark 3.1.9** If product quality constraints are re-added to Problem P-3.1.5, then Theorem 3.1.8 still applies, with valid input dominance breakpoints  $\mathcal{B}_I \cap [P^L, P^U]$ .

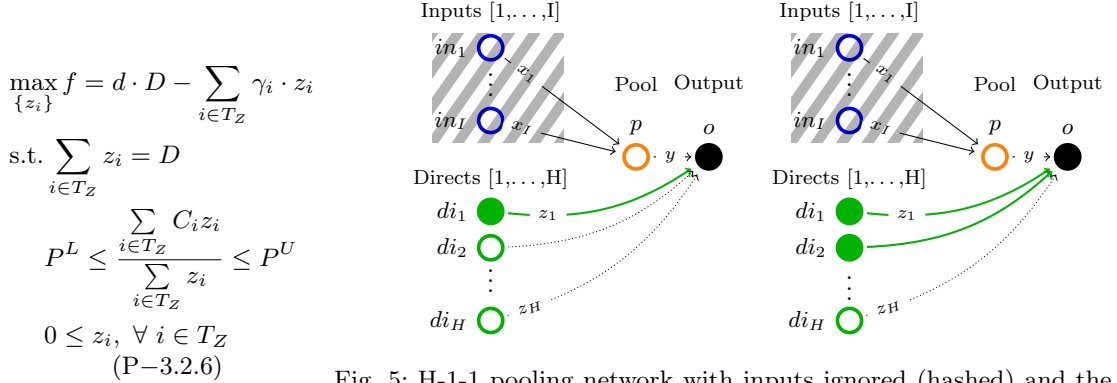
We conclude the I-1-1 sub-case analysis with a numerical example showcasing the implications of Theorem 3.1.8. For the Fig. 4 example with five inputs and no quality constraints, the function  $f^*(p)$  reveals breakpoints at concentrations  $C_2, C_3$  and  $C_4$  in a piecewise-linear structure, as expected via Lemma 3.1.1. Furthermore, the dominant input active sets are sparse, since at any  $p$  they involve at most a pair of inputs and consequently a pair of non-zero flow variables. The coupling of sparsity with piecewise-linear structure matches the Beale et al. [8] intuition. These special structures provide motivation to further explore  $p$ -parametric optimal objective structure on progressively more general problem sub-instances in the remaining sections.

### 3.2 Directs-Only Analysis (H-1-1 Sub-Case)

This subsection restricts Problem P-3.4 to disallow flows from the input nodes to the pool node ( $x_i = 0, \forall i \in T_X$ ). The resulting Problem P-3.2.6, which is complementary to Section 3.1, also



incorporates the product quality constraints. Optimal solutions implying direct-only flows are not parametric on  $p$ , since the problem is independent of pool concentration. This subsection therefore seeks the unique, dominant direct active set and its solution. Lemmas 3.2.1–3.2.2 give feasibility results. Given an active set, Definition 3.2.3 introduces the output concentration obtained at the optimum of Problem P–3.4. The optimal output concentration proves essential by creating links and a domination ordering among all direct active sets via Lemma 3.2.4, Corollary 3.2.7, Lemma 3.2.8. With a domination ordering, Theorem 3.2.9 finds the optimal direct-only solution and the dominant direct active set. It is well known that Problem P–3.2.6 is a single linear program [59], but the following analysis is important because the feasibility and output concentration results developed in this subsection will be central to the Section 3.3 analysis.



**Lemma 3.2.1** (Simple feasibility conditions)

- (i) A feasible direct active set (solution) exists  $\Leftrightarrow \exists i \in T_Z$  s.t.  $P^L \leq C_i \leq P^U$  or  $\exists i, j \in T_Z$  s.t.  $C_i < P^L, C_j > P^U$ .
- (ii) An direct active pair  $\{i, j\}$  is feasible  $\Leftrightarrow i$  and  $j$  are feasible or  $(P^U - C_i)(P^U - C_j) < 0$  or  $(P^L - C_i)(P^L - C_j) < 0$ .

*Proof* (i) If  $\exists i \in T_Z$  s.t.  $P^L \leq C_i \leq P^U$  then Problem P-3.2.6 is obviously feasible. Alternatively, w.l.o.g., if  $C_i < P^L$ , there must  $\exists j \in T_Z$  with  $C_j > P^L$  so an output concentration within  $[P^L, P^U]$  can be obtained. However, this case implicitly assumed  $\exists i \in T_Z$  s.t.  $P^L \leq C_i \leq P^U$ , and consequently  $C_j > P^U$ , concluding the proof.

(ii) Both  $(P^U - C_i)(P^U - C_j) < 0$  or  $(P^L - C_i)(P^L - C_j) < 0$  imply  $C_i$  and  $C_j$  are on opposite sides of a product quality bound and thus the linear combination of their concentrations implied by active  $\{i, j\}$  can be within  $[P^L, P^U]$ , making  $\{i, j\}$  feasible.  $\square$

**Lemma 3.2.2** (*Pair dominating both its individual nodes and feasibility*)

If  $\{i, j\}$  is a feasible direct active pair, then:

$$\{i, j\} \succeq i, j \Leftrightarrow \alpha = \arg \min_{i, j} (\gamma_i, \gamma_j) \text{ is infeasible, i.e. } C_\alpha \notin [P^L, P^U].$$

*Proof* '⇒': If both  $C_i, C_j \in [P^L, P^U]$ , then  $\arg \min_{i, j} (\gamma_i, \gamma_j) \succeq \{i, j\}$ , contradiction, so we can assume w.l.o.g.  $C_i \notin [P^L, P^U]$ . If also  $C_j \notin [P^L, P^U]$  both  $i$  and  $j$  are infeasible alone, but  $\{i, j\}$  can be feasible if the second condition in Lemma 3.2.1.i is met. In the previous case, one of the nodes  $i, j$  has the properties needed. Else if  $C_j \in [P^L, P^U]$  and  $\gamma_i > \gamma_j$ , then  $j \succeq \{i, j\}$  - therefore  $\gamma_i < \gamma_j$ . The reverse proof '⇐' is trivial.  $\square$

**Definition 3.2.3** For a feasible direct active pair  $\{i, j\}$  with  $\{i, j\} \succeq i, j$ , denote by  $P(i, j)$  the output concentration at optimality for Problem P-3.2.6, depending on properties of  $i, j$  via:

$$P(i, j) = \left( \frac{P^U + P^L}{2} \right) - \left( \frac{P^U - P^L}{2} \right) \cdot \text{sgn}((C_i - C_j)(\gamma_i - \gamma_j)) = \begin{cases} P^L, & \text{if } (C_i - C_j)(\gamma_i - \gamma_j) > 0 \\ P^U, & \text{if } (C_i - C_j)(\gamma_i - \gamma_j) < 0. \end{cases} \quad (19)$$

Note that due to Remark 3.5 and Lemmas 3.2.1-3.2.2 we have  $(C_i - C_j)(\gamma_i - \gamma_j) \neq 0$ .

**Lemma 3.2.4** (*Optimal output concentration for sets not trivially dominated*)

- (i) For a feasible direct active pair  $\{i, j\}$  with  $\{i, j\} \succeq i, j$ , the optimal output concentration equals a quality bound, i.e.  $(C_i z_i + C_j z_j) / (z_i + z_j) = P(i, j)$ .
- (ii) A feasible direct active triple  $\{i, j, k\}$ , with a subset  $\{i, j\} \succeq i, j$ , delivers output concentration  $(C_i z_i + C_j z_j + C_k z_k) / (z_i + z_j + z_k) = P(i, j)$  or else is trivially dominated by a subset.
- (iii) A feasible direct active set  $N = \{d_1, \dots, d_n\}$ ,  $n > 2$ , with a subset  $\{d_1, d_2\} \succeq d_1, d_2$ , delivers output concentration  $\sum_{i \in N} C_i z_i / \sum_{i \in N} z_i = P(d_1, d_2)$  or else is trivially dominated by a subset.

*Proof* (i)-(ii) Proofs in Appendix A.

(iii) The proof proceeds by induction, with the base case proven in Item ii. Assume the assertion holds for up to  $n$  nodes to prove it holds for  $n + 1$  nodes. Split set  $N$  in two distinct subsets, with  $N_l \cap N_r = \emptyset$ ,  $N_l \cup N_r = N$  and aggregate the nodes in  $N_l$  and  $N_r$  as single joint nodes  $l$  and  $r$ , respectively, with:

$$z_\alpha = \sum_{i \in N_\alpha} z_i, \quad \gamma_\alpha = \sum_{i \in N_\alpha} \gamma_i z_i / \sum_{i \in N_\alpha} z_i, \quad C_\alpha = \sum_{i \in N_\alpha} C_i z_i / \sum_{i \in N_\alpha} z_i, \quad \forall \alpha \in \{l, r\}.$$

Then either  $\{l, r\} \succeq l, r$  or else active set  $N$  is trivially dominated by a subset,  $N_l$  or  $N_r$ .

If, for example,  $\{l, r\} \preceq l$  then, according to the reverse of Lemma 3.2.2,  $l$  must be feasible and  $\gamma_l < \gamma_r$ . If the additional node  $d_{n+1}$  has  $\gamma_{d_{n+1}} < \gamma_r$ , then adding node  $r$  to pair  $\{l, d_{n+1}\}$  ( $\{l, d_{n+1}\}$  can be viewed as a single feasible node since  $l$  is feasible) contradicts the condition in Lemma 3.2.2, and implies  $\{l, r, d_{n+1}\} \preceq \{l, d_{n+1}\}$ . Else, if  $\gamma_{d_{n+1}} > \gamma_r$ , node  $d_{n+1}$  only increases overall cost by being active so  $\{l, r, d_{n+1}\} \preceq \{l, r\}$ . Thus, in all cases where  $\{l, r\} \preceq l$ ,  $\{d_1, \dots, d_n, d_{n+1}\}$  is trivially dominated by a subset. The same would hold for  $\{l, r\} \preceq r$ .

Alternatively, if  $\{l, r\} \succeq l, r$  and  $N$  is not trivially dominated by a subset, then Item **ii** applies to the triple  $\{l, r, d_{n+1}\}$ . Since in this case, by inductive assumption,  $\sum_{i \in N} C_i z_i / \sum_{i \in N} z_i = (C_l z_l + C_r z_r) / (z_l + z_r) = P(d_1, d_2)$ , then Item **ii** implies  $(C_l z_l + C_r z_r + C_{d_{n+1}} z_{d_{n+1}}) / (z_l + z_r + z_{d_{n+1}}) = P(d_1, d_2)$ , as needed.  $\square$

**Remark 3.2.5** The result in Lemma 3.2.4.i implies that for a feasible direct active pair  $\{i, j\}$  with  $\{i, j\} \succeq i, j$ , Problem P–3.2.6 becomes:

$$\begin{aligned} \max_{z_i, z_j} f &= d \cdot D - \gamma_i \cdot z_i - \gamma_j \cdot z_j \\ \text{s.t. } z_i + z_j &= D \\ P(i, j) &= (C_i z_i + C_j z_j) / (z_i + z_j) \\ 0 < z_i, z_j. \end{aligned} \tag{P-3.2.7}$$

Problem P–3.2.7 is analogous to the input-only Problem P–3.1.5, with input flows  $x_i$  replaced by direct flows  $z_i$  and fixed pool concentration  $p$  replaced by a product quality limit  $P(i, j)$  (either lower or upper). Thus, the flow and dominance results for pairs in Section 3.1 are mirrored via Corollaries 3.2.6–3.2.7. Moreover, any pair viable as the dominant direct active set needs to first dominate both its individual nodes, so only such pairs and their solutions are of interest.

The results in Lemma 3.2.4 further allow a common fixed output concentration as common reference between different direct active sets. Thus, the fixed output concentration plays the same role in obtaining the dominance results in Lemma 3.2.8 as the fixed pool concentration  $p$  in obtaining Lemma 3.1.5 and Lemma 3.1.6 for the inputs-only analysis.

**Corollary 3.2.6** The flows of a feasible direct active pair  $\{i, j\}$  in Problem P–3.2.7 are:

$$z_i = \frac{D(P(i, j) - C_j)}{C_i - C_j}, \quad z_j = \frac{D(P(i, j) - C_i)}{C_j - C_i}. \tag{20}$$

*Proof* Analogous to Lemma 3.1.1, but for Problem P–3.2.7 rather than Problem P–3.1.5.  $\square$

**Corollary 3.2.7** (*Domination condition between active direct pairs*)

For  $i, j, k, l \in T_Z$  with  $\{i, j\}, \{k, l\}$  feasible,  $ij = \{i, j\} \succ kl = \{k, l\} \Leftrightarrow$

$$P(i, j) \left( \frac{\gamma_i - \gamma_j}{C_i - C_j} \right) + \frac{\gamma_j C_i - \gamma_i C_j}{C_i - C_j} < P(k, l) \left( \frac{\gamma_k - \gamma_l}{C_k - C_l} \right) + \frac{\gamma_l C_k - \gamma_k C_l}{C_k - C_l} \Leftrightarrow \tag{21a}$$

$$\frac{\gamma_i(P(i, j) - C_j) + \gamma_j(C_i - P(i, j))}{C_i - C_j} = \gamma_{ij} < \gamma_{kl} = \frac{\gamma_k(P(k, l) - C_l) + \gamma_l(C_k - P(k, l))}{C_k - C_l}. \tag{21b}$$

*Proof* Analogous to Proposition 3.1.3, but for Problem P–3.2.7 rather than Problem P–3.1.5.  $\square$

**Lemma 3.2.8** If a feasible direct active pair  $\{i, j\}$ , with  $\{i, j\} \succeq i, j$  also dominates all other feasible direct pairs then:

- (i)  $\{i, j\}$  dominates any feasible direct triple  $\{i, j, k\} \forall k \in T_Z$ .
- (ii)  $\{i, j\}$  dominates any direct node set of any higher cardinality.

*Proof* (i) Proof in Appendix A.

(ii) The proof proceeds analogously to Lemma 3.1.6.ii, with direct instead of input flows,  $P(i, j)$  instead of  $p$ , and Item **i** as the base case.  $\square$

**Theorem 3.2.9** (*Directs-only optimal solution and dominant direct active set*)

Given  $\{i, j\}$  a feasible direct active pair that dominates any such alternative pairs, i.e.:

$$\{i, j\} = \arg \min_{\substack{\text{feasible } \{k, l\} \subseteq T_Z, \\ \{k, l\} \succeq k, l}} \gamma_{kl} = \arg \min_{\substack{\text{feasible } \{k, l\} \subseteq T_Z, \\ \{k, l\} \succeq k, l}} \frac{\gamma_k(P(k, l) - C_l) + \gamma_l(C_k - P(k, l))}{C_k - C_l}, \quad (22)$$

which can be found in strongly-polynomial time  $O(H^2)$ , then either:

- a) If  $\{i, j\} \succeq i, j$  then  $\mathcal{A}_D = \{i, j\}$  with the flows in Eq. (20) and  $f^* = D \cdot (d - \gamma_{ij})$ .
- b) Else,  $\mathcal{A}_D = \alpha = \arg \min_{\alpha \in \{i, j\}} \gamma_\alpha$  with  $z_\alpha = D$  and  $f^* = D \cdot (d - \gamma_\alpha)$ .

*Proof* Eq. (22) follows directly from Corollary 3.2.7.

a) If  $\{i, j\} \succeq i, j$ , Lemma 3.2.2 implies one of the nodes, w.l.o.g  $j$ , is infeasible, so w.l.o.g  $C_j > P^U, C_i < P^U$  and  $\gamma_j < \gamma_i$ . If  $\exists k \in T_Z \setminus \{i\}$  s.t.  $C_k < P^U, \gamma_k < \gamma_i$ , then  $\{k, j\} \succeq \{i, j\}$ , contradiction. Therefore (feasible)  $i$  dominates any other alternative feasible direct, and by transitivity,  $\{i, j\} \succeq i \succeq k \forall k \in T_Z \setminus \{i\}, C_k \in [P^L, P^U]$ . The latter together with Lemma 3.2.8 implies that  $\{i, j\}$  is the dominant direct active set.

b) Assume  $i \succeq \{i, j\}$ , so  $i$  is feasible with  $P^L \leq C_i \leq P^U$ . If  $\gamma_j < \gamma_i$  then  $\{i, j\}$  as a pair with a linearly weighted cost would dominate  $i$ , contradiction, and therefore  $\gamma_j > \gamma_i$ . If more restrictively,  $P^L < C_i < P^U$ , since by transitivity  $i \succeq \{i, j\} \succeq \{i, k\} \forall k \in T_Z \setminus \{i, j\}$  ( $\{i, k\}$  feasible due to  $P^L < C_i < P^U$ ), therefore  $\gamma_k > \gamma_i \forall k \in T_Z \setminus \{i\}$  and  $\mathcal{A}_D = i$ . Now the complementary restriction of  $C_i = P^U$  is assumed ( $C_i = P^L$  is analogous). If  $\exists k \in T_Z \setminus \{j\}, C_k < P^U, \gamma_k < \gamma_i$  then  $\{i, k\} \succeq i \succeq \{i, j\}$ , contradiction, therefore  $\forall k \in T_Z \setminus \{j\}, C_k < P^U$  we have  $\gamma_k > \gamma_i$ . Additionally, since  $\{i, j\}$  feasible implies  $C_j < P^U$ , if  $\exists k \in T_Z$  s.t.  $C_k > P^U, \gamma_k < \gamma_i$  then  $\{k, j\} \succeq \{i, j\}$ , contradiction, thus  $\forall k \in T_Z, C_k > P^U, \gamma_k > \gamma_i$ . Therefore, all sub-cases after assuming  $i \succeq \{i, j\}$  result in  $\mathcal{A}_D = i$ .  $\square$

### 3.3 Inputs and Directs Analysis (I+H-1-1 Instance)

This subsection considers the original  $p$ -parametric Problem P-3.4, allowing mixed active sets of both input and direct nodes. Theorem 3.3.1 uses the interplay of earlier results for both input (Section 3.1) and direct (Section 3.2) active sets to pinpoint mixed active sets that can be dominant (overall) active sets as triples of two inputs and one direct. This section focusses on mixed triples not dominated by the dominant input active set  $\mathcal{A}_I$ . Definition 3.3.2 first extends the feasibility conditions from Section 3.2 for mixed triples viewed as direct pairs to  $p$ -intervals by partitioning any  $p$ -interval  $\Phi$  around  $\{P^L, P^U\}$  if necessary and building  $Q(\Phi)$ , the set of directs making the mixed active set feasible. Definition 3.3.2.e also extends the directs domination result in Lemma 3.2.2 to  $p$ -intervals. Lastly, Definition 3.3.2.f splits  $p$ -intervals  $\Phi$  into sub-intervals  $\Phi_I$  and  $\Phi_M$  based on whether the dominant mixed active triple is dominated or not by  $\mathcal{A}_I$  over the sub-intervals, respectively. Using the breakpoints between mixed and input active sets identified in Lemma 3.3.3, Lemma 3.3.4 then implements the  $\Phi_I/\Phi_M$  split of any interval  $\Phi$ .

Based on the latter results, Proposition 3.3.5 finds the dominant mixed active set for fixed  $p$  and all mixed dominance breakpoints, while Proposition 3.3.6 finds all dominance breakpoints. Moreover, Proposition 3.3.7 finds the  $p$ -parametric optimal objective function to be monotone convex/concave for mixed active sets. Consequently, Theorem 3.3.8 summarizes all cases of optimal objective monotonicity. Finally, Theorem 3.3.9 uses all objective monotonicity results to find the optimal solution at a breakpoint dominance point in strongly-polynomial time.

**Theorem 3.3.1** (*Dominant mixed active set that can dominate overall at fixed  $p$  and its flows*)

For fixed  $p$  and  $i, j \in T_X, \mathcal{A}_I(p) = \{i, j\} = ij$  (as in Section 3.1, with no product quality constraints)

$\Rightarrow \mathcal{A}_M(p) = \{i, j, q\}$ ,  $q \in T_Z$ , with flow solutions,

$$x_i = \frac{D(p - C_j)(P(ij, q) - C_q)}{(C_i - C_j)(p - C_q)}, \quad x_j = \frac{D(p - C_i)(P(ij, q) - C_q)}{(C_j - C_i)(p - C_q)}, \quad z_q = \frac{D(p - P(ij, q))}{(p - C_q)}, \quad (23)$$

or else  $\mathcal{A}_M(p) \preceq_p \mathcal{A}_I(p)$ .

*Proof* Fixing  $p$ , the concentration the active input set delivers via the pool towards the output concentration, implies product quality constraints on output concentration become irrelevant when considering only the active inputs part of a mixed active set. This observation allows to first pre-solve the inputs-only sub-Problem P–3.3.8, where the objective function  $f_A(p, x_A(p))$  is now also parametric on variable total input flow  $x_A(p)$  for an active input set  $A$ . According to Corollary 3.1.7,  $A = ij = \{i, j\}$  at optimality for Problem P–3.3.8, with the solution in Eq. (25).

$$\begin{aligned} \max_{\{x_i | i \in A\}} f_A(p, x_A(p)) &= d \cdot x_A(p) - \sum_{i \in A} \gamma_i \cdot x_i & \mathcal{A}_I(p) &= \{i, j\} = ij \\ \text{s.t. } \sum_{i \in A} x_i &= x_A(p) & f_A^*(p, x_A(p)) &= f_{ij}(p, x_{ij}(p)) \\ & & &= d \cdot x_{ij}(p) - \gamma_{ij}(p) \cdot x_{ij}(p) \\ p &= \sum_{i \in A} C_i x_i / \sum_{i \in A} x_i & \text{Section 3.1} & \Rightarrow & x_i &= \frac{x_{ij}(p)(p - C_j)}{C_i - C_j} \\ 0 \leq x_i, \forall i \in A \subseteq T_X & & & & x_j &= \frac{x_{ij}(p)(p - C_i)}{C_j - C_i} \end{aligned} \quad (\text{P-3.3.8}) \quad (25)$$

Now the optimal input-only parametric solution in Eq. (25) can be incorporated into the full Problem P–3.4. This results in a direct-only Problem P–3.3.9 that is augmented by the active joint input node  $ij$  acting via the pool as an active (additional) direct node with fixed concentration  $p$  and variable flow  $x_{ij}(p)$ . Denote the dominant direct active set for the augmented Problem P–3.3.9 at fixed  $p$  with  $\mathcal{A}_D^p$  and note that Problem P–3.3.9 accounts for any possible dominant mixed active set  $\mathcal{A}_M(p)$ . Applying Theorem 3.2.9 to Problem P–3.3.9 and taking into account  $ij$  must be active implies that, given  $\{ij, q\} \succeq_p \{ij, l\} \forall l \in T_Z$ ,  $\{ij, l\}$  feasible and  $p$  fixed, if  $\{ij, q\} \succeq_p ij$  then  $\mathcal{A}_D^p = \{ij, q\} = \mathcal{A}_M(p)$  or else  $\mathcal{A}_D^p = ij = \mathcal{A}_I(p) \succeq_p \mathcal{A}_M(p)$ . Therefore, a mixed active set can be the overall dominant active set if  $\mathcal{A}_D^p = \{ij, q\} = \mathcal{A}_M(p)$  and Eq. (27a) is the solution to Problem P–3.3.9.

$$\begin{aligned} \max_{\{z_k\}, x_{ij}(p)} f(p) &= d \cdot D - \gamma_{ij}(p) \cdot x_{ij}(p) - \sum_{i \in T_Z} \gamma_k \cdot z_k & \left\{ \begin{array}{l} \mathcal{A}_D^p = \{ij, q\} = \mathcal{A}_M(p) \\ f^*(p) = f_{\{ij, q\}}(p) \\ x_{ij}(p) = \frac{D(P(ij, q) - C_q)}{p - C_q} \\ z_q = \frac{D(p - P(ij, q))}{p - C_q} \end{array} \right. & (27a) \\ \text{s.t. } \sum_{k \in T_Z} z_k + x_{ij}(p) &= D & \text{Section 3.2} & \Rightarrow & & \\ P^L \cdot D \leq \sum_{k \in T_Z} C_k z_k + p \cdot x_{ij}(p) &\leq P^U \cdot D & & & & \\ 0 \leq z_k \forall k \in T_Z, \quad 0 < x_{ij}(p) &\text{ for } i, j \in T_X, & \text{or} & & & \\ & (\text{P-3.3.9}) & & & \mathcal{A}_D^p = \mathcal{A}_I(p) = ij \succeq_p \mathcal{A}_M(p) & (27b) \end{aligned}$$

Finally, the flow solutions in Eq. (23) are found by combining Eq. (25) with Eq. (27a).  $\square$

**Definition 3.3.2** (*Feasibility/domination extensions to  $p$ -intervals around quality bounds*)

(a) Let sub-intervals of the partition  $\{P^L, P^U\}$  of inputs/directs concentrations be denoted by:

$$\begin{aligned} I_L^X &= [\min_{i \in T_X} C_i, P^L], & I_U^X &= (P^U, \max_{i \in T_X} C_i], \\ I_L^Z &= [\min_{i \in T_Z} C_i, P^L], & I_U^Z &= (P^U, \max_{i \in T_Z} C_i]. \end{aligned} \quad I_{LU} = [P^L, P^U],$$



- (b) Let  $\Phi \subseteq [C_i, C_j]$  denote a closed  $p$ -interval between two consecutive input dominance breakpoints, i.e.  $C_i, C_j \in \mathcal{B}_I$ ,  $\mathcal{B}_I \cap (C_i, C_j) = \emptyset$ , with  $(\forall p \in \Phi) \mathcal{A}_I(p) = ij$ . Let  $\Phi \in \{[C_i, C_j] \cap I_L^X, [C_i, C_j] \cap I_{LU}, [C_i, C_j] \cap I_U^X\}$  such that:

$$\mathbb{1}_{\Phi \subseteq I_L^X} + \mathbb{1}_{\Phi \subseteq I_{LU}} + \mathbb{1}_{\Phi \subseteq I_U^X} = 1.$$

- (c) Let  $Q(\Phi)$  be the set of directs with concentration outside  $\Phi$ 's partition around  $\{P^L, P^U\}$ , i.e.:

$$\begin{aligned} Q(\Phi) &= \{q \in T_Z \mid C_q \in [\min_{i \in T_Z} C_i, \max_{i \in T_Z} C_i] \setminus I_\beta^Z, \text{ where } \Phi \subseteq I_\beta^X, \beta \in \{L, LU, U\}\} \\ &= \{q \in T_Z \mid \text{mixed active set } \{ij, q\} \text{ is feasible, where } (\forall p \in \Phi) \mathcal{A}_I(p) = ij\}. \end{aligned}$$

- (d) Let  $R(\Phi) \subseteq Q(\Phi)$  denote a subset s.t.  $(\forall q \in R(\Phi))(\forall p \in \Phi) \gamma_q < \gamma_{ij}(p)$ . Since  $\gamma_{ij}(p)$ , as defined in Eq. (8), is a linear function of  $p$  with extremes at  $\Phi$  endpoints,

$$R(\Phi) = \{q \in Q(\Phi) \mid \gamma_q < \max\{\gamma_{ij}(b_l), \gamma_{ij}(b_u)\}, \text{ where } \Phi = [b_l, b_u]\},$$

- (e) Let  $\Theta(\Phi) = \begin{cases} R(\Phi) & \text{if } R(\Phi) \neq \emptyset \text{ or } \Phi \subseteq I_{LU}, \\ Q(\Phi) & \text{if } R(\Phi) = \emptyset \text{ and } \Phi \not\subseteq I_{LU}. \end{cases}$

- (f) Let  $\Phi_I, \Phi_M$  be partition sub-intervals of  $\Phi$ , where  $\mathcal{A}_I, \mathcal{A}_M$  dominate, respectively. Assuming  $(\forall p \in \Phi) \mathcal{A}_I(p) = ij$ ,

$$\begin{aligned} \Phi_I &= \{p \in \Phi \mid (\forall q \in \Theta(\Phi)) \gamma_{ij}(p) \leq \gamma_q \Rightarrow \text{if } \Phi \subseteq I_{LU} \text{ then } (\forall q) ij \succeq_p \{ij, q\}, \mathcal{A}_I(p) \succeq_p \mathcal{A}_M(p)\}, \\ \Phi_M &= \{p \in \Phi \mid (\exists q \in \Theta(\Phi)) \gamma_{ij}(p) \geq \gamma_q \Leftrightarrow (\exists q \in \Theta(\Phi)) ij \preceq_p \{ij, q\} \Leftrightarrow \mathcal{A}_I(p) \preceq_p \mathcal{A}_M(p)\}. \end{aligned} \quad (28)$$

Thus,  $\Theta(\Phi)$  extends Lemmas 3.2.1 and 3.2.2 from fixed  $p$  to interval  $\Phi$  (see proof of Lemma 3.3.4.i).

**Lemma 3.3.3** (*Domination/breakpoints between dominant input and mixed active sets*)

If  $i, j \in T_X$ ,  $q \in T_Z$ , then  $ij = \{i, j\} \preceq_p \{ij, q\} = \{i, j, q\} \Leftrightarrow$

$$\gamma_{ij}(p) \geq \gamma_q \Leftrightarrow \gamma_{ij}(p) \geq \gamma_{\{ij, q\}}(p) := \frac{\gamma_q(P(ij, q) - p) + \gamma_{ij}(p)(C_q - P(ij, q))}{C_q - p}, \quad (29)$$

with  $\{i, j\} \succ_p \{i, j, q\}$  at breakpoint pool concentration  $p = \frac{C_i(\gamma_q - \gamma_j) - C_j(\gamma_q - \gamma_i)}{\gamma_i - \gamma_j}$ .

*Proof* Proof in Appendix A. □

**Lemma 3.3.4** For a given  $p$ -interval  $\Phi = [b_l, b_u]$ , where  $b_l, b_u \in \mathcal{B}_I \cup \{C_i, C_j\}$ ,  $(\forall p \in \Phi) \mathcal{A}_I(p) = ij$ , we have:

- (i)  $(\forall p \in \Phi) (\mathcal{A}_M(p) = \{ij, q\} \Rightarrow q \in \Theta(\Phi))$ .  
 (ii)  $(\forall \Phi)$  Sub-intervals  $\Phi_I, \Phi_M$  can be found explicitly as:

$$\begin{cases} (a) \Phi_I = \Phi, \Phi_M = \emptyset, \text{ if } \Theta(\Phi) = \emptyset, \\ (b) \Phi_I = \{p \in \Phi \mid b_l \leq p \leq \min(S)\}, \Phi_M = \{p \in \Phi \mid \min(S) \leq p \leq b_u\}, \text{ else if } \frac{\gamma_i - \gamma_j}{C_i - C_j} > 0, \\ (c) \Phi_I = \{p \in \Phi \mid \max(S) \leq p \leq b_u\}, \Phi_M = \{p \in \Phi \mid b_l \leq p \leq \max(S)\}, \text{ else if } \frac{\gamma_i - \gamma_j}{C_i - C_j} < 0, \end{cases} \quad (30)$$

where:

$$S = \{p \mid \{i, j\} \succ_p \{i, j, q\}, \forall q \in \Theta(\Phi)\} = \left\{ \frac{C_i(\gamma_q - \gamma_j) - C_j(\gamma_q - \gamma_i)}{\gamma_i - \gamma_j} \mid \forall q \in \Theta(\Phi) \right\}. \quad (31)$$

(iii)  $(\forall q \in \Theta(\Phi))(\forall p \in \hat{\Phi} \in \{\Phi_I, \Phi_M\})$  if  $\mathcal{A}_M(p) = \{ij, q\}$  then  $P(ij, q)$  reduces to:

$$P(ij, q) = \begin{cases} P^L, & \text{if } ((C_q < b_u) \oplus (\hat{\Phi} = \Phi_M)) \wedge (P^L - C_q)(P^L - b_u) < 0, \\ P^U, & \text{if } ((C_q > b_u) \oplus (\hat{\Phi} = \Phi_M)) \wedge (P^U - C_q)(P^U - b_u) < 0, \end{cases} \quad (32)$$

independent of specific  $p \in \hat{\Phi}$ .

*Proof* (i) The restriction  $Q(\Phi) \in T_Z$ , and its subset  $R(\Phi) \in T_Z$ , enforces Lemma 3.2.1 feasibility for  $\{ij, q\}$ ,  $\forall p \in \Phi$  viewed as a direct active set. Set  $\Theta(\Phi)$  also enforces the Lemma 3.2.2 domination condition  $\{ij, q\} \succeq_p ij \Leftrightarrow \forall p \in \Phi \gamma_q \leq \gamma_{ij}(p)$  via  $\Theta(\Phi) = R(\Phi)$ . When  $R(\Phi) = \emptyset$  and  $\Phi \subseteq I_{LU}$  then  $ij$  feasible and  $(\forall q \in Q(\Phi))(\forall p \in \Phi) \gamma_q \geq \gamma_{ij}(p) \Leftrightarrow (\forall p \in \Phi) ij \succeq \mathcal{A}_M(p)$ , in which case  $\Theta(\Phi) = R(\Phi) = \emptyset$  since  $(\forall p \in \Phi) \mathcal{A}_M(p) \neq \mathcal{A}^*(p)$ . When  $R(\Phi) = \emptyset$  and  $\Phi \not\subseteq I_{LU}$  then  $ij$  infeasible, and since a direct needs to be active for feasibility, in this case  $\Theta(\Phi) = Q(\Phi)$  and  $(\forall q \in Q(\Phi))(\forall p \in \Phi) \gamma_q \geq \gamma_{ij}(p)$  but  $\{ij, q\} \not\succeq_p ij, q$ . Therefore in this case,  $\Theta(\Phi)$  is extended from  $R(\Phi)$  to  $Q(\Phi)$ .

(ii) Case (a) results by construction of  $\Phi_I, \Phi_M, \Theta(\Phi)$ . For Case (b)-(c),  $S$  is built as the set of all breakpoints from Lemma 3.3.3 where  $\gamma_{ij}(p) = \gamma_q, \forall p \in S, q \in \Theta(\Phi)$ . From Eq. (8),  $\partial\gamma_{ij}(p)/\partial p = (\gamma_i - \gamma_j)/(C_i - C_j)$ , which implies if  $\partial\gamma_{ij}(p)/\partial p > 0$  then  $\gamma_{ij}(p)$  is increasing with  $p$ . Therefore, given  $\forall b \in S, \gamma_{ij}(b) = \gamma_q$ , if  $\partial\gamma_{ij}(p)/\partial p > 0$  then  $\forall p \leq b \gamma_{ij}(p) \leq \gamma_q$  and vice-versa. Consequently, if  $\partial\gamma_{ij}(p)/\partial p > 0$  then  $\Phi_I$  is the restriction of  $\Phi$  up till  $\min(S)$ , and otherwise  $\Phi_I$  is the restriction of  $\Phi$  from  $\max(S)$ .

Consequently,  $\forall p \in \Phi_I$ , if  $ij$  is feasible ( $\Phi \subseteq I_{LU}$ ) then  $ij$  dominates any mixed active set  $\{ij, q\}$  and Theorem 3.3.1 then implies  $(\forall p \in \Phi_I) \mathcal{A}_I(p) \succeq_p \mathcal{A}_M(p)$ . Complementary,  $\{ij, q\}$  is feasible by construction ( $q \in \Theta(\Phi)$ ), and therefore  $\forall p \in \Phi_M \exists q \in \Theta(\Phi) \gamma_{ij}(p) \geq \gamma_q \Leftrightarrow \exists q \in \Theta(\Phi) ij \preceq_p \{ij, q\} \Leftrightarrow \mathcal{A}_I(p) \preceq_p \mathcal{A}_M(p)$ .

(iii) Assume first  $\hat{\Phi} = \Phi_I \neq \Phi_M$ . Then, Eq. (28) implies  $(\forall q \in \Theta(\Phi))(\forall p \in \hat{\Phi}) \gamma_{ij}(p) \leq \gamma_q$ . Consequently, the expression for  $P(ij, q)$  according to Definition 3.2.3 reduces to Eq. (32). Now assume  $\hat{\Phi} = \Phi_M \neq \Phi_I$ . Then, Eq. (28) implies  $(\forall p \in \hat{\Phi}) \mathcal{A}_M(p) = \{ij, q\} \succeq_p \mathcal{A}_I(p)$  and hence  $(\forall p \in \hat{\Phi}) \gamma_{ij}(p) \geq \gamma_q$ . Thus, again, the expression for  $P(ij, q)$  reduces to Eq. (32). For both possible  $\hat{\Phi} \in \{\Phi_I, \Phi_M\}$ , due to the construction of  $\Phi$  and  $\Theta(\Phi)$  with  $q \in \Theta(\Phi)$ ,  $(\forall p \in \hat{\Phi}) (C_q < p) = (C_q < b_u)$ , and thus the comparison becomes independent of a specific  $p \in \hat{\Phi}$ . Furthermore, to ensure feasibility of  $\{ij, q\}$  according to Lemma 3.2.1.ii,  $(P(ij, q) - C_q)(P(ij, q) - b_u) < 0$  is enforced explicitly in Eq. (32).  $\square$

**Proposition 3.3.5** For  $\hat{\Phi} = [b_l, b_u] \in \{\Phi_M; \Phi_I \not\subseteq I_{LU}\} \subseteq \Phi$ ,  $(\forall p \in \Phi) \mathcal{A}_I(p) = ij$ ,  $Q(\Phi) \neq \emptyset$ :

(i) (The dominant mixed active set at  $p$ ) For fixed  $p \in \hat{\Phi}$ ,  $\mathcal{A}_M(p) = \{ij, q\} \succeq_p \mathcal{A}_I(p)$  with

$$q = \arg \min_{r \in \Theta(\Phi)} \left( \gamma_{\{ij, r\}}(p) := \frac{\gamma_r(P(ij, r) - p) + \gamma_{ij}(p)(C_r - P(ij, r))}{C_r - p} \right). \quad (33)$$

(ii) (The set of mixed dominance breakpoints over  $\hat{\Phi}$ )

$$\begin{aligned} \mathcal{B}_M &\supseteq \left\{ p \in \text{int } \hat{\Phi} \mid \{ij, q\} \succ_p \{ij, r\} \wedge q, r \in \mathcal{A}_M(p), \forall q, r \in \Theta(\Phi) \right\} \\ &= \left\{ p \in \text{int } \hat{\Phi} \mid p \in \text{SqrRoots}(\Gamma(p, P(ij, q), P(ij, r))) \wedge q, r \in \mathcal{A}_M(p), \forall q, r \in \Theta(\Phi) \right\}, \end{aligned} \quad (34)$$

with  $(\forall q \in \Theta(\Phi)) P(ij, q)$  as in Eq. (32) and independent of  $p$ ;  $b_l, b_u \in \mathcal{B}_M$  as well.

*Proof* (i) If  $\hat{\Phi} \not\subseteq I_{LU}$ , then  $\mathcal{A}_I(p) = ij$  is infeasible and by default  $\mathcal{A}_M(p) \succeq_p \mathcal{A}_I(p)$ . If  $\hat{\Phi} = \Phi_M$ , then, from the construction of  $\Phi_M$  in Eq. (28),  $\mathcal{A}_M(p) \succeq_p \mathcal{A}_I(p)$ . Thus Theorem 3.3.1 asserts via Eq. (27a) that  $\mathcal{A}_D^p = \{ij, q\} = \mathcal{A}_M(p)$  for a  $q \in \Theta(\Phi)$ , as required by Lemma 3.3.4.i. By viewing  $\{ij, q\}$  as a dominant direct pair with  $ij$  active in order to find  $\mathcal{A}_D^p$ , the condition Eq. (22)

in Theorem 3.2.9 becomes Eq. (33). Since  $p$  is fixed, Eq. (33) can be solved using the original Definition 3.2.3 for  $P(ij, q) \forall q \in \Theta(\Phi)$ .

(ii) Appendix A proves Eq. (34) and introduces function  $\Gamma(p, P(ij, q), P(ij, r))$  which is quadratic in  $p$  and linear in  $P(ij, q), P(ij, r)$ . To solve the function  $\Gamma(p, P(ij, q), P(ij, r))$  as a quadratic of  $p$ , ( $\forall q \in \Theta(\Phi)$ )  $P(ij, q)$  has to be independent of  $p$  via the form in Eq. (32). First, Lemma 3.3.4.iii implies  $\forall p \in \hat{\Phi}$  that if  $\{ij, q\} = \mathcal{A}_M(p)$  then  $P(ij, q)$  in Eq. (32) is correct; therefore any dominant breakpoint within  $\Phi$  between  $\{ij, q\}$  and another dominant mixed set is captured in  $\mathcal{B}_M$ . Second, Lemma 3.3.4.iii implies if Eq. (32)  $\neq$  Definition 3.2.3 for  $P(ij, q)$ ,  $q \in \Theta(\Phi)$ , then feasible  $\{ij, q\} \neq \mathcal{A}_M(p)$ . Consequently, the conjunctive condition  $q, r \in \mathcal{A}_M(p)$  eliminates not only those mixed breakpoints that are not dominant, but also those calculated on potentially incorrect  $P(ij, q)$  from Eq. (32). Note that, unlike the inputs-only case of Section 3.1, two breakpoints between any  $\{ij, q\}$  and  $\{ij, r\}$  can occur, because  $f_{\{ij, q\}}(p)$  and  $f_{\{ij, r\}}(p)$  are convex or concave functions (see Proposition 3.3.7) which can intersect at two points. The endpoints of  $\hat{\Phi}$  also represent mixed dominance breakpoints, since for  $p \in \{b_l, b_u\}$ , given  $\mathcal{A}_M(p) = \{ij, q\}$ , either  $ij, q$  or  $P(ij, q)$  change at  $p$ , creating a breakpoint.  $\square$

**Proposition 3.3.6** For a  $p$ -interval  $\Phi = [b_l, b_u]$ , ( $\forall p \in \Phi$ )  $\mathcal{A}_I(p) = ij$ :

(a) ( $\forall p \in \Phi_I \subseteq I_{LU}$ ),  $ij$  feasible and  $\mathcal{A}^*(p) \in \{\mathcal{A}_I(p), \mathcal{A}_D\}$  with dominance breakpoint

$$\left\{ p \in \Phi_I \mid ij \succ_p \mathcal{A}_D := \alpha \Leftrightarrow \gamma_{ij}(p) = \gamma_\alpha \Leftrightarrow p = \frac{C_i(\gamma_q - \gamma_j) - C_j(\gamma_q - \gamma_i)}{\gamma_i - \gamma_j} \right\} \subseteq \mathcal{B}. \quad (35)$$

(b) ( $\forall p \in \hat{\Phi}$ ), for  $\hat{\Phi} \in \{\Phi_M; \Phi_I \not\subseteq I_{LU}\} \subseteq \Phi$ ,  $\mathcal{A}^*(p) \in \{\mathcal{A}_D, \mathcal{A}_M(p)\}$  with dominance breakpoints

$$\left\{ p \in \hat{\Phi} \mid (\{ij, q\} \succ_p \mathcal{A}_D := \alpha \Leftrightarrow p = b_{\{ij, q\}, \alpha}) \wedge q \in \mathcal{A}_M(p), \forall q \in \Theta(\Phi) \right\} \subseteq \mathcal{B}$$

where  $b_{\{ij, q\}, \alpha} = \frac{(C_i - C_j)(\gamma_\alpha C_q - P(ij, q)\gamma_q) + (C_q - P(ij, q))(\gamma_j C_i - \gamma_i C_j)}{(C_i - C_j)(\gamma_\alpha - \gamma_q) + (C_q - P(ij, q))(\gamma_i - \gamma_j)}$ ,  $P(ij, q)$  as in Eq. (32).

*Proof* (a) By construction, ( $\forall p \in \Phi_I \subseteq I_{LU}$ )  $\mathcal{A}_I(p) \succeq_p \mathcal{A}_M(p)$  and thus  $\mathcal{A}^*(p) \in \{ij, \mathcal{A}_D\}$ . The breakpoint in Eq. (35) follows directly from Lemma 3.3.3.

(b) The breakpoint condition in Eq. (36) is similar to the one of Lemma 3.3.3, but with the input active set replaced by  $\mathcal{A}_D = \alpha$ . The associated dominance breakpoint  $b_{\{ij, q\}, \alpha}$  is also found analogously as in Lemma 3.3.3 (details omitted for brevity). The use of the  $p$ -independent expression for  $P(ij, q)$  in Eq. (32) for every  $q \in \Theta(\Phi)$  is justified by the same arguments as in the proof for Proposition 3.3.5.ii (mixed set only on one side of any potential breakpoint).  $\square$

**Proposition 3.3.7** (*Derivatives of objective function w.r.t.  $p$  and convex/monotone properties*)  
For fixed  $p$  and mixed active triple  $A = \{i, j, q\} = \{ij, q\}$ ,  $i, j \in T_X$ ,  $q \in T_Z$  in Problem P-3.4,

$$\frac{\partial^n f_A}{\partial p^n} = (-1)^n n! \frac{D(P(ij, q) - C_q)}{(C_i - C_j)(p - C_q)^{n+1}} \cdot \left( C_q(\gamma_j - \gamma_i) + C_j(\gamma_i - \gamma_q) + C_i(\gamma_q - \gamma_j) \right), \quad (37)$$

which implies  $f_A(p)$  is monotone convex/concave:

- If  $p > C_q$  then  $\text{sgn}(\frac{\partial f_A}{\partial p}) \neq \text{sgn}(\frac{\partial^2 f_A}{\partial p^2})$  and  $f_A(p)$  is concave increasing or convex decreasing.
- If  $p < C_q$  then  $\text{sgn}(\frac{\partial f_A}{\partial p}) = \text{sgn}(\frac{\partial^2 f_A}{\partial p^2})$  and  $f_A(p)$  is concave decreasing or convex increasing.

*Proof* Proof in Appendix A.  $\square$

**Theorem 3.3.8** ( *$p$ -Parametric structure of the optimal objective function  $f^*(p)$* )

Consider a given  $p$ -interval  $\Phi$  between two consecutive dominance breakpoints for Problem P-3.4. Functions  $f^*$ ,  $\mathcal{A}^*$ ,  $\mathcal{A}_I$ ,  $\mathcal{A}_M$  are  $p$ -parametric with the following cases,

- (a) (direct)  $(\forall p \in \Phi) \mathcal{A}^*(p) = \mathcal{A}_D = \{l, r\}$  or  $r \Rightarrow f^*|_{\Phi}(p)$  is constant,
- (b) (input)  $(\forall p \in \Phi) \mathcal{A}^*(p) = \mathcal{A}_I(p) = ij \Rightarrow f^*|_{\Phi}(p)$  is linear,
- (c) (mixed)  $(\forall p \in \Phi) \mathcal{A}^*(p) = \mathcal{A}_M(p) = \{ij, q\} \Rightarrow f^*|_{\Phi}(p)$  is monotone convex/concave,

where  $(\forall p \in \Phi) i, j \in T_X, l, r, q \in T_Z$  are fixed.

*Proof* Case (a) follows from Theorem 3.2.9 and the independence of the results therein w.r.t.  $p$ ; Case (b) from Lemma 3.1.1 and Corollary 3.1.7; Case 3 from Theorem 3.3.1 and Proposition 3.3.7.  $\square$

**Theorem 3.3.9** (*Optimal solution and dominance breakpoints for I+H-1-1 instance*)

For Problem P–3.4, let  $\mathcal{B}_{IM} \in B_I \cup B_M$  and exclude from  $\mathcal{B}_{IM}$  any redundant breakpoints with the same active sets on both sides. Then

$$f^* = \max \left( \max_{p \in \mathcal{B}_{IM}} f^*(p), f_{\mathcal{A}_D}^* \right), \quad (38)$$

with the optimal objective value  $f_{\mathcal{A}_D}^*$  for the dominant direct active set acting as a threshold. Both  $f^*$  and a full description of  $f^*(p)$  via all dominance breakpoints  $\mathcal{B}$  ( $\mathcal{B}_{IM}$  plus all dominance breakpoints with  $\mathcal{A}_D$ ) can be obtained in strongly-polynomial time  $O(I^3 + H^3)$ . Also,

*Proof* Denoting by  $T(\cdot)$  the time-complexity of calculating result  $(\cdot)$ ,

$$\begin{aligned} T(f^*) &= T(\mathcal{B}_I) + T(\mathcal{B}_M) + T(\mathcal{A}_D) = T(\text{Eq. (18a)}) + T(\text{Eq. (34)}) + T(\text{Eq. (22)}) \\ &= O(I^3) + O(H^3) + O(H^2) = O(I^3 + H^3). \end{aligned} \quad (39)$$

Eq. (34) can be solved in  $O(H^3)$  because all mixed dominance breakpoints for all  $p$ -intervals  $\Phi$  can be found in one pass of complexity  $O(H^3)$  and then assigned to each  $p$ -interval. Since  $T(\text{Eq. (36)}) + T(\text{Eq. (35)}) = O(H^2)$ ,  $T(\mathcal{B}) = T(f^*)$ .  $\square$

Fig. 6 illustrates the I+H-1-1 instance with a numerical example showcasing the implications of Theorem 3.3.8. For a chosen parametrization of five inputs (same inputs as in Fig. 4) and three directs with quality constraints, the  $p$ -parametric function  $f^*(p)$  reveals additional breakpoints compared to Fig. 4 between mixed and input active sets and between mixed and direct active sets. The structure is still piecewise-monotone, but is extended to piecewise  $p$ -intervals exhibiting convexity or concavity, e.g. when  $3 \leq p \leq 4$  where mixed active set  $\{in_3, in_3, di_1\}$  is dominant.

Similar to the results in Section 3.1, the coupling between the piecewise structure and sparse active sets (up to a mixed node triple) is still present, allowing a full description of the  $p$ -parametric optimal solution space. Section 4 explicitly uses this full description to find optimal solutions in strongly-polynomial time for a multiple outputs instance.

**Remark 3.3.10** (*Assumptions: Analytical solutions/sparsity/piecewise structure versus LP*)

This section finds analytically the optimal solution for a I+H-1-1 pooling topology with Assumption 2.2, going beyond the obvious LP black-box Problem P–3.4 to identify active feeds sparsity and piecewise-monotonicity of the  $p$ -parametric optimal objective  $f^*(p)$ . Relaxing feasibility or fixed product demand  $D$  implies either an infeasible or unprofitable problem with all feeds inactive and  $f^* = 0$ , or the same solution with product demand reaching its upper limit.

However, reinstating constraints on feed availability will erode solution sparsity proportionately to tightness of the flow bounds on dominant feeds. For fixed  $p$ , if the dominant active set reaches its upper flow bounds, the next-in-line dominant active set would send flow and so on, recursively. If the bounds on cheaper feeds are very tight, this effect would create a hierarchy of dominant active sets participating in the solution. Therefore, the tighter the flow bounds, the more active feeds, and the less sparsity. Piecewise function  $f^*(p)$  would hence have more breakpoints accounting for

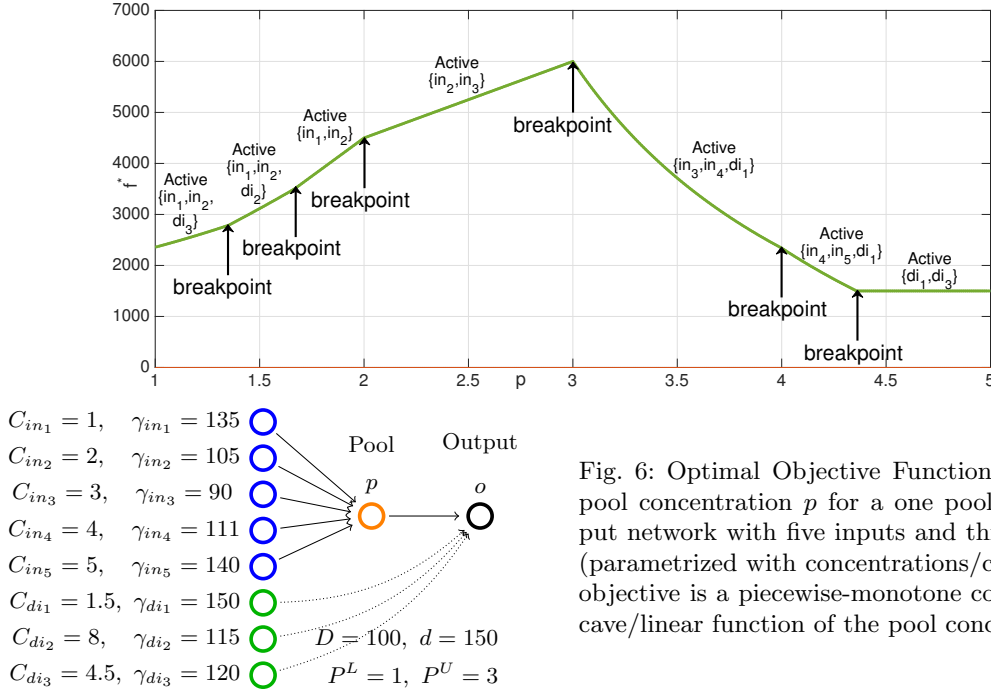


Fig. 6: Optimal Objective Function  $f^*(p)$  vs. pool concentration  $p$  for a one pool, one output network with five inputs and three directs (parametrized with concentrations/costs). The objective is a piecewise-monotone convex/concave/linear function of the pool concentration.

dominance relations and optimal balancing between all active sets in the dominance hierarchy, not just the top active set. Moreover, because  $f^*(p)$  would represent an addition over a hierarchy of active sets,  $f^*(p)$  can be piecewise non-monotone as in Section 4. Equally importantly, balancing the flows among the hierarchy of dominant active sets under flow constraints is an inherent LP, not solvable analytically. The dominant active set cardinality also increases proportionally with the number of qualities in order to meet tougher feasibility conditions for multiple qualities.

In conclusion, for feed flow bounds or multiple qualities, sparsity and piecewise parametric objective structure both vanish and the I+H-1-1 instance can only be solved using LP. Section 3.3 hence marks the boundary of topological/ $p$ -parametric structure present in the I+H-1-1 instance.

#### 4 Instance I+H-1-J: One Pool, Multiple Outputs

This section extends the analysis in Section 3 with Assumption 2.2 to  $I + H$  feeds ( $I$  inputs,  $H$  directs), one pool and multiple  $J$  outputs. Again, for simplicity of notation, single index  $l$  is dropped via the notation transformations  $T_X \leftarrow \{i : (i, l) \in T_X\}$ ,  $T_Y \leftarrow \{j : (l, j) \in T_Y\}$ . This leads to Problem P-4.10, where surplus variables  $y_j \forall j \in \overline{1, J} \setminus T_Y$  are introduced and set to 0 as a surplus condition. Note that eliminating  $p$  and  $y_j \forall j \in T_Y$  from Problem P-4.10 does not produce a linear program as in Section 3, but instead a bilinear problem that can be non-convex.

To analyse Problem P-4.10, Theorem 4.1 first proves its equivalence to Problem P-4.11. The result allows additively decomposing Problem P-4.11 over outputs into sub-problems P-4.11- $j$ , which are all  $p$ -parametric and equivalent to I+H-1-1 instances studied in Section 3. Definition 4.2 then extends dominance breakpoints and dominant active sets for a multiple outputs problem setting. Proposition 4.3 shows that the composed master Problem P-4.11 can present  $p$ -parametric non-monotonicity or non-convexity on specific  $p$ -intervals. This hurdle is cleared by Theorem 4.4, which finds in polynomial time all stationary points on non-monotone breakpoint intervals by solv-

ing a univariate rational polynomial. Finally, Corollary 4.5 offers a strongly-polynomial worst-case time complexity for solving Problem P–4.11 to optimality. The section concludes by Remark 4.6

$$\begin{aligned}
& \max_{\substack{\{x_i\}, \{y_j\}, \\ \{z_{i,j}\}, p}} f = \sum_{j \in \overline{1, J}} d_j \cdot y_j + \sum_{(i,j) \in T_Z} d_j \cdot z_{i,j} - \sum_{i \in T_X} \gamma_i \cdot x_i - \sum_{(i,j) \in T_Z} \gamma_i \cdot z_{i,j} \\
& \text{s.t. } y_j + \sum_{i: (i,j) \in T_Z} z_{i,j} = D_j \quad \forall j \in \overline{1, J} \\
& \sum_{i \in T_X} x_i - \sum_{j \in \overline{1, J}} y_j = 0 \\
& P_j^L \leq \left( p \cdot y_j + \sum_{i: (i,j) \in T_Z} C_i \cdot z_{i,j} \right) / \left( y_j + \sum_{i: (i,j) \in T_Z} z_{i,j} \right) \leq P_j^U \quad \forall j \in \overline{1, J} \quad (\text{P-4.10}) \\
& \sum_{i \in T_X} C_i x_i = p \sum_{j \in \overline{1, J}} y_j \\
& 0 \leq x_i \quad \forall i \in T_X \quad \quad 0 \leq y_j \quad \forall j \in T_Y \quad \quad 0 \leq z_{i,j} \quad \forall (i,j) \in T_Z \\
& \quad \quad \quad \quad \quad \quad 0 = y_j \quad \forall j \in \overline{1, J} \setminus T_Y
\end{aligned}$$

**Theorem 4.1** (*p-Parametric additive decomposition over multiple outputs*)

As visualized in Fig. 7, Problem P–4.10 can be reformulated as a Problem P–4.11 of maximizing the total sum of  $J$   $p$ -parametric optimal objectives over  $p$ , each associated to a one output subproblem P–4.11– $j$  (same type as Problem P–3.4).

$$\max_p f^*(p) = \max_p \left( \sum_{j \in \overline{1, J}} f_j^*(p) \right) \quad (\text{P-4.11})$$

$$\text{with } x_i = \sum_{j \in \overline{1, J}} x_{i,j} \quad \forall i \in T_X, \quad y_j = \sum_{i \in T_X} x_{i,j} \quad \forall j \in \overline{1, J}, \quad p = \sum_{i \in T_X} C_i x_i / \sum_{j \in \overline{1, J}} y_j$$

$$\text{s.t. } \forall j \in \overline{1, J} \left\{ \begin{array}{l} f_j^*(p) = \max_{\{x_{i,j}\}, \{z_{i,j}\}} f_j(p) \\ f_j(p) = d_j \cdot D_j - \sum_{i \in T_X} \gamma_i \cdot x_{i,j} - \sum_{i \in T_Z} \gamma_i \cdot z_{i,j} \\ \text{s.t. } \sum_{i \in T_X} x_{i,j} + \sum_{i \in T_Z} z_{i,j} = D_j \\ P_j^L \leq \left( \sum_{i \in T_X} C_i x_{i,j} + \sum_{i \in T_Z} C_i z_{i,j} \right) / D_j \leq P_j^U \\ p = \sum_{i \in T_X} C_i x_{i,j} / \sum_{i \in T_X} x_{i,j} \\ 0 \leq x_{i,j} \quad \forall i \in T_X, j \in T_Y \quad \quad 0 \leq z_{i,j}, \quad \forall (i,j) \in T_Z \\ 0 = x_{i,j} \quad \forall i \in T_X, j \notin T_Y \end{array} \right.$$

(P–4.11– $j$ )

*Proof* Each  $x_i \quad \forall i \in T_X$  can be split into a sum of flows  $x_{i,j} \quad \forall j \in \overline{1, J}$ , with each  $x_{i,j}$  representing the flow output  $j$  gets via the pool from input  $i$ . This allows similar output-based splits for the two constraints in Problem P–4.10 that apply jointly over all outputs, i.e. flow and quality balance:

$$x_i = \sum_{j \in \overline{1, J}} x_{i,j} \quad \forall i \in T_X \quad \Rightarrow \quad \sum_{i \in T_X} x_{i,j} - y_j = 0 \quad \forall j \in \overline{1, J}, \quad \sum_{i \in T_X} C_i x_{i,j} = p \cdot y_j \quad \forall j \in \overline{1, J}.$$

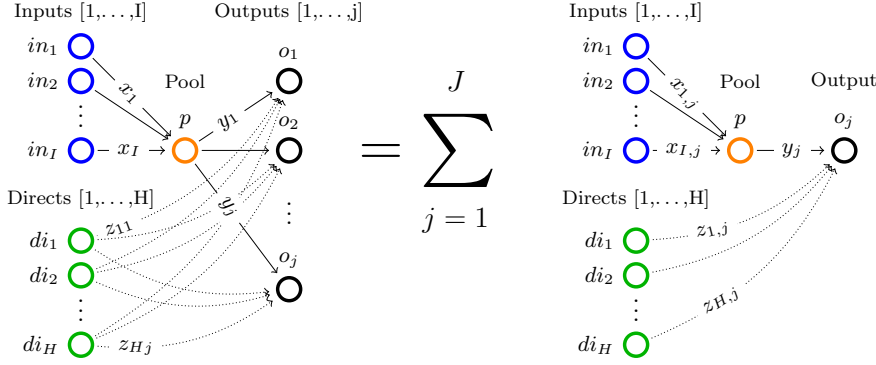


Fig. 7:  $p$ -Parametric additive decomposition of a multiple outputs problem into a sum of one output problems based on which output feed flows arrive at.

Furthermore, the objective  $f$  as a function of  $p$  in Problem P-4.10 can be rewritten as,

$$f(p) = \sum_{j \in \overline{1, J}} \left( d_j \cdot y_j + \sum_{i: (i, j) \in T_Z} d_j \cdot z_{i, j} - \sum_{i \in T_X} \gamma_i \cdot x_{i, j} - \sum_{i: (i, j) \in T_Z} \gamma_i \cdot z_{i, j} \right) := \sum_{j \in \overline{1, J}} f_j(p),$$

where each  $f_j$  contains a different set of variables and parameters for a fixed  $j$  except for common variable  $p$  which it is parametrized on. In the context of maximizing  $f(p)$ , we have:

$$\begin{aligned} \max_{\{x_i\}, \{y_j\}, \{z_{i, j}\}, p} f &= \max_p \left( \max_{\{x_i\}, \{y_j\}, \{z_{i, j}\}} f(p) \right) = \max_p \left( \max_{\{x_{i, j}\}, \{y_j\}, \{z_{i, j}\}} f(p) \right) \\ &= \max_p \left( \max_{\{x_{i, j}\}, \{y_j\}, \{z_{i, j}\}} \sum_{j \in \overline{1, J}} f_j(p) \right) = \max_p \left( \sum_{j \in \overline{1, J}} \max_{\{x_{i, j}\}, \{z_{i, j}\}} f_j(p) \right) = \max_p \left( \sum_{j \in \overline{1, J}} f_j^*(p) \right), \end{aligned}$$

Finally, separating out both the objective and constraints parts for all  $j \in \overline{1, J}$  from Problem P-4.10, we obtain a collection of  $J$  sub-problems P-4.11- $j$ , all parametric on and therefore linked via a common  $p$  but otherwise independent. However, as shown in Section 3.3, each  $p$ -parametric sub-problem P-4.11- $j$  can be solved analytically using the piecewise structure of  $f_j^*(p)$ , and each solution can be used directly towards solving the master Problem P-4.10 linking all  $J$  sub-problems. Note that, for each sub-problem P-4.11- $j \forall j \in \overline{1, J}$ ,  $y_j$  is eliminated as in Problem P-3.4, with the surplus condition enforced through the  $x$  variables set to 0; when  $j \notin T_Y$ , the sub-problem is thus a directs-only one. □

**Definition 4.2** (*Dominance breakpoints and dominant active sets*)

- Let  $\mathcal{B}_J = \bigcup_{j \in \overline{1, J}} \mathcal{B}_j$  be the joint dominance breakpoint set for Problem P-4.11- $j$  over all  $J$  outputs/sub-problems, with  $\mathcal{B}_j$  the dominance breakpoints set for the  $j$ -th sub-problem P-4.11- $j$ , found as in Section 3.
- Let  $\Phi_J$  denote any closed interval with two consecutive elements in  $\mathcal{B}_J$  as endpoints.
- Let  $\mathcal{A}_j^*(p)$  denote the dominant active set at  $p$  for the  $j$ -th sub-problem P-4.11- $j$ , as found in Theorem 3.3.8; by construction,  $\mathcal{A}_j^*(p)$  remains constant over  $\Phi_J$  s.t.  $\forall p \in \Phi_J \mathcal{A}_j^*(p) = \mathcal{A}_j^*(\Phi_J)$ .

**Proposition 4.3** In Problem P-4.11, for  $\forall p \in \Phi_J$ ,  $f^*(p)$  can be non-monotone or non-convex.

*Proof* From Theorem 3.3.8, for a given  $\Phi_J$ , ( $\forall j \in \overline{1, J}$ ) ( $\forall p \in \Phi_J$ )  $f_j^*(p)$  can be either constant, linear or monotone convex/concave depending on dominant active set  $\mathcal{A}_j^*(\Phi_J)$ . Consider a two-output Problem P-4.11 with,

$$f^*(p) = f_1^*(p) = f_{j_1}^*(p) + f_{j_2}^*(p),$$

and  $f_{j_1}^*(p)$  concave increasing and  $f_{j_2}^*(p)$  concave decreasing. Then

$$\exists p_1 \in \text{int}(\Phi_J) \text{ s.t. } \frac{\partial f^*(p)}{\partial p} = \frac{\partial f_{j_1}^*(p)}{\partial p} + \frac{\partial f_{j_2}^*(p)}{\partial p} = 0,$$

meaning  $f^*(p)$  has a local maximum at  $p_1$  and is non-monotone. Now consider a four-output Problem P-4.11 with  $f^*(p) = f_1^*(p) + f_2^*(p)$  with  $f_2^*(p)$  constructed analogously as  $f_1^*(p)$  but having a local maximum at  $p_2 \in \Phi_J$ ,  $p_2 \neq p_1$ . In this case,  $f^*(p)$  is multi-modal with at least two local maxima and therefore non-convex.  $\square$

**Theorem 4.4** Assuming Problem P-4.11 has all parameters rational, given interval  $\Phi_J$ , then finding  $f^*|_{\Phi_J} = \max_{p \in \Phi_J}(f^*(p))$  requires finding all stationary points of  $f^*(p)$  over  $\Phi_J$  by solving a univariate rational polynomial of maximum degree  $2 \cdot |T_Y|$ , i.e.:

$$\frac{\partial f^*(p)}{\partial p} = \left( \sum_{\substack{j \in T_Y, \\ \text{s.t. } \mathcal{A}_j^* = \{i, k, q\} \\ i, k \in T_X, (q, j) \in T_Z}} \frac{D_j(C_q - P(ik, q))}{(C_i - C_k)(p - C_q)^2} \cdot (C_q(\gamma_k - \gamma_i) + C_k(\gamma_i - \gamma_q) + C_i(\gamma_q - \gamma_k)) \right) + C = 0, \quad (41)$$

where  $C$  is a constant. The polynomial in Eq. (41) can be solved in strongly-polynomial time with respect to  $T_Y$ ,  $|T_Y| \leq J$ .

*Proof* Section 3 implies that for Problem P-4.11,

$$\begin{aligned} \frac{\partial f^*(p)}{\partial p} &= \sum_{j \in \overline{1, J}} \frac{\partial f_j^*(p)}{\partial p} \stackrel{\text{Section 3.2}}{=} \sum_{j \in T_Y} \frac{\partial f_j^*(p)}{\partial p} \\ &= \sum_{\substack{j \in T_Y, \\ \text{s.t. } \mathcal{A}_j^* = \{i, k, q\} \\ i, k \in T_X, (q, j) \in T_Z}} \frac{\partial f_j^*(p)}{\partial p} + \sum_{\substack{j \in T_Y, \\ \text{s.t. } \mathcal{A}_j^* = \{i, k\} \\ i, k \in T_X}} \frac{\partial f_j^*(p)}{\partial p} \stackrel{\substack{\text{Theorem 3.3.8,} \\ \text{Lemma 3.1.1}}}{=} \text{Eq. (41)}. \end{aligned} \quad (42)$$

The value  $f^*|_{\Phi_J}$  corresponds to the maximum objective function value evaluated at all stationary points. To find all roots/stationary points of  $f^*(p) \forall p \in \Phi_J$ , the common denominator can be multiplied out in Eq. (41) to form a polynomial. The resulting polynomial from Eq. (41) will have maximum degree  $2 \cdot |T_Y|$  if  $\forall j \in T_Y$   $\mathcal{A}_j^*(\Phi_J) = \{i, k, q\}$ ,  $i, k \in T_X$ ,  $(q, j) \in T_Z$  and if  $q_1 \neq q_2$  given  $q_1 \in \mathcal{A}_{j_1}^*(\Phi_J)$ ,  $q_2 \in \mathcal{A}_{j_2}^*(\Phi_J)$ ,  $(q_1, j), (q_2, j) \in T_Z$ . Furthermore, by assumption, the polynomial in Eq. (41) has rational coefficients. Consequently,

$$\frac{\partial f^*(p)}{\partial p} = \sum_{0 \leq i \leq 2\hat{J}, \hat{j} \leq T_Y} a_i \cdot p^i, \quad \forall i \ a_i \in \mathbb{Q}, \quad (43)$$

which according to the deterministic *Lenstra-Lenstra-Lovacs* algorithm [37] can be solved with a strongly-polynomial worst-case time bound  $T(\text{Poly-LLL})$ ,

$$T(\text{Poly-LLL}) = O \left( (2|T_Y|)^{12} + (2|T_Y|)^9 \left( \log \left| \frac{\partial f^*(p)}{\partial p} \right| \right)^3 \right), \text{ where } \left| \frac{\partial f^*(p)}{\partial p} \right| = \left( \sum_i a_i^2 \right)^{1/2}. \quad (44)$$

$\square$



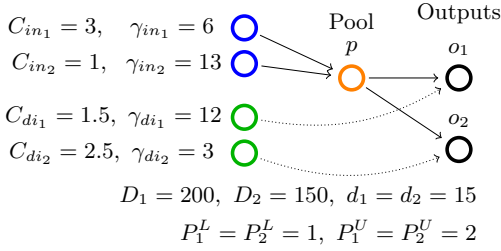
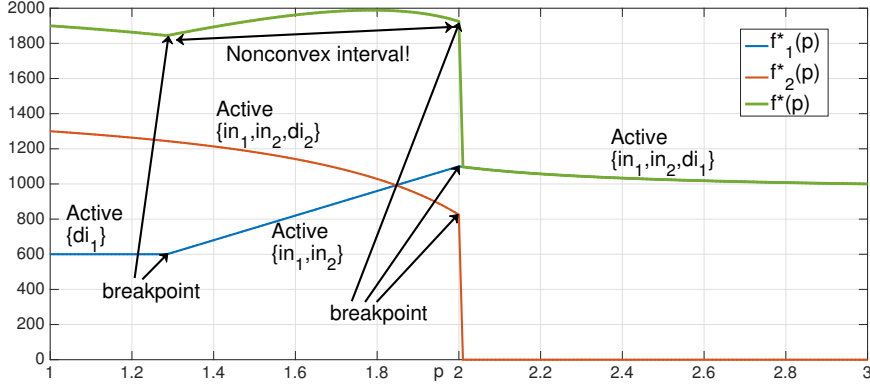


Fig. 8: Optimal Objective Function  $f^*(p)$  vs. pool concentration  $p$  for a one pool, two-output network with two inputs and two directs (parametrized with concentrations/costs). The objective  $f^*(p) = f_1^*(p) + f_2^*(p)$  is a sum of the objectives corresponding one output sub-problems, and is a piecewise (possibly non-monotone/non-convex) function of the pool concentration.

**Corollary 4.5** (Strongly-polynomial time complexity)

Problem P-4.11  $\Leftrightarrow$  Problem P-4.10 with all parameters rational is solved in strongly-polynomial worst-case time

$$O((I^3 + H^3) \cdot J) + O(I \cdot H^2) \cdot (O(\text{Poly-LLL}) + O(J)), \tag{45}$$

where  $O(\text{Poly-LLL})$  is polynomial w.r.t.  $|T_Y| < J$  (see Theorem 4.4, Eq. (44)).

*Proof* In the worst case, on all intervals between two joint dominance breakpoints in  $\mathcal{B}_J$  the additive decomposition over outputs in Problem P-4.11 requires solving a univariate rational polynomial as in Theorem 4.4. Denoting by  $T(\cdot)$  the time-complexity of calculating result  $(\cdot)$ , this implies

$$\begin{aligned}
 T(f^*) &= T(\mathcal{B}_J) + O(|\mathcal{B}_J|) \cdot (O(\text{Poly-LLL}) + O(J)) \\
 &= O(I^3 + H^3) \cdot O(J) + O(|\mathcal{B}_J|) \cdot O(\text{Poly-LLL}).
 \end{aligned}
 \tag{46}$$

Eq. (46) accounts for both the size of  $\mathcal{B}_J$  and the time to find  $\mathcal{B}_J$  assuming for simplicity  $|T_Y| = J$ . Eq. (46) also includes objective evaluations at maximum  $J$  stationary points found after applying Theorem 4.4 (time  $O(\text{Poly-LLL})$ ) for any breakpoint interval. Furthermore, due to Theorem 3.3.9,  $\max |\mathcal{B}_J| \Rightarrow \max |\mathcal{B}_{IM}|$  when all breakpoints between input and mixed sets are dominant. Assuming a breakpoint between the dominant mixed/input set and the dominant direct set on any interval between two consecutive elements of  $\mathcal{B}_{IM}$  does not change the order of  $|\mathcal{B}_{IM}|$ . Therefore,

$$O(|\mathcal{B}_J|) = O(|\mathcal{B}_{IM}|) = O(|\mathcal{B}_I|) \cdot O(|\mathcal{B}_M|) = O(I \cdot H^2), \tag{47}$$

since on each interval between two input dominance breakpoints there can be mixed dominance breakpoints between a pair of mixed sets, therefore between a pair of directs (see Proposition 3.3.5). Finally, combining Eqs. (46) and (47) results in Eq. (45).  $\square$

Fig. 8 illustrates the I+H-1-J instance analysis with a numerical example showcasing the implications of Proposition 4.3 and Theorem 4.4. For a chosen parametrization of two inputs, directs

and outputs with quality constraints for each output in Fig. 8, the  $p$ -parametric function  $f^*(p)$  is decomposed additively in the optimal objectives of the one output sub-problems. Hence, in the particular example,  $f^*(p)$  has a non-monotone piecewise section as proven in Proposition 4.3 for  $p \in (1.3, 2)$  with a stationary point which can be deterministically found via Theorem 4.4.

**Remark 4.6** (*A new  $P/NP$  boundary point for standard pooling*)

The Section 4 results address a gap in the literature for the  $P/NP$  boundary for standard pooling problems. The time-complexity gap [4, Corollary 2] occurs between I+H-L-J instances with one quality that are strongly  $NP$ -hard and I-1-J instances with a bounded number of qualities that are  $P$ -hard. Theorem 4.4 and Corollary 4.5 show that instances I+H-1-J with one quality and restricted by Assumption 2.2 are strongly-polynomial. If, however, any of  $D_j \forall j \in T_Y$  are not fixed but unknown, then Eq. (41) becomes a multivariate rational polynomial which is  $NP$ -hard to solve [24]. Similarly, re-introducing feeds flow bounds, for any particular  $j \in T_Y$ , the mixed active set term in Eq. (41) gets split into a hierarchy of potential mixed active sets (see Remark 3.3.10) each with total flow an unknown proportion of  $D_j$ ; this again leads to a multivariate polynomial. Furthermore, if multiple qualities  $K$  are introduced then variables  $p_k, k \in \overline{1, K}$ , are not independent - a specific pool concentration in one quality restricts the concentration range in another quality. Consequently, Eq. (41) becomes a  $NP$ -hard multivariate polynomial system. Lastly, for full topology I+H-L-J with Assumption 2.2, again Eq. (41) becomes a coupled multivariate system when two pools send non-zero flow to the same output - see Section 5, Theorem 5.2.

In summary, when feed to output connections (directs) are considered, the instance I+H-1-J with Assumption 2.2 lies on the  $P/NP$  boundary, and can be solved analytically as shown in this section despite having  $f^*(p)$  being piecewise non-monotone or non-convex.

**Remark 4.7** (*Haverly [32] is strongly-polynomially solvable*) The Haverly [32] instances, i.e. the first set of three pooling problems in the literature are single-quality, I+H-1-J instances following Assumption 2.2. We can obtain their exact solutions analytically in strongly-polynomial time!

**Remark 4.8** (*Connection to queueing theory*) Woodside and Tripathi [60] report similar, piecewise-monotone structure in a central processor queueing problem where workstation files are assigned to file servers. The Woodside and Tripathi [60] proofs cannot be directly applied to standard pooling, but the similarity recalls the deep connection between pooling and queueing.

## 5 Instance I+H-L-1: Multiple Pools, One Output

This section extends the analysis in Section 3 with Assumption 2.2 to  $I + H$  feeds ( $I$  inputs,  $H$  directs),  $L$  pools and one output. Again, for simplicity of notation, single index  $j$  is dropped via the notation transformations  $T_Z \leftarrow \{i : (i, j) \in T_Z\}$ ,  $T_Y \leftarrow \{l : (l, j) \in T_Y\}$ . This leads to Problem P-5.12, where eliminating variables  $p_l, y_l \forall l \in T_Y$  results in an LP with a black-box solution as for Problem P-3.4 in Section 3. We further identify this solution analytically, understanding pool sparsity and the parametric structure of the optimal objective in the process.

To analyse Problem P-5.12, Definition 5.1 first introduces active pools. Theorem 5.2 then finds a maximum of two active pools contribute to the optimal solution and further shows all cases induced are parametric on pools concentrations. Furthermore, Theorem 5.3 proves all cases involved in Theorem 5.2 in fact reduce to I+H-1-1 problem instances studied in Section 3. Finally, Corollary 5.4 offers a strongly-polynomial bound on solving Problem P-5.12 and the section concludes with an illustrative numerical example.

**Definition 5.1** (*Active pools*)

- Let the  $L = |T_Y|$  pools in Problem P-5.12 be denoted by  $i$  with concentration  $p_i, \forall i \in \overline{1, L}$ .

- An active pool has incoming and outgoing flows strictly non-zero. A non-active pool  $l \in T_Y$  has well-defined concentration by assuming only  $y_l = 0$  but  $x_{i,l} \neq 0$ ,  $\forall i : (i, l) \in T_X$ . However, any non-active pool is disconnected via  $y_l = 0$  from the output, does not influence objective function  $f$ , and can be removed along with any of its flow connections from Problem P–5.12.

$$\begin{aligned}
 \max_{\substack{\{x_{i,l}\}, \{y_l\}, \\ \{z_i\}, \{p_l\}}} \quad & f = \sum_{l \in T_Y} d \cdot y_l + \sum_{i \in T_Z} d \cdot z_i - \sum_{(i,l) \in T_X} \gamma_i \cdot x_{i,l} - \sum_{i \in T_Z} \gamma_i \cdot z_i \\
 \text{s.t.} \quad & \sum_{l \in T_Y} y_l + \sum_{i \in T_Z} z_i = D \\
 & \sum_{i:(i,l) \in T_X} x_{i,l} - y_l = 0 \quad \forall l \\
 & P^L \cdot D \leq \sum_{l \in T_Y} p_l \cdot y_l + \sum_{i \in T_Z} C_i \cdot z_i \leq P^U \cdot D \\
 & \sum_{i:(i,l) \in T_X} C_i x_{i,l} = p_l y_l \quad \forall l \\
 & 0 \leq x_{i,l} \quad \forall (i, l) \in T_X, \quad 0 \leq y_l \quad \forall l \in T_Y, \quad 0 \leq z_i \quad \forall i \in T_Z
 \end{aligned} \tag{P-5.12}$$

**Theorem 5.2** (*Pool sparsity and pool-parametric objective function*)

For fixed  $p_l \quad \forall l \in T_Y$ , at optimality, Problem P–5.12 has a maximum of two active pools with the optimal objective function parametric on their concentrations:

$$\max_{\substack{\{x_{i,l}\}, \{y_l\}, \\ \{z_i\}, \{p_l\}}} f = \begin{cases} \max_{\{x_{i,m}\}, \{x_{i,n}\}} f(p_m, p_n), & \text{if } m, n \in T_Y \text{ active, } T_Y \setminus \{m, n\} \text{ not active,} \\ \max_{\{x_{i,m}\}, \{z_i\}} f(p_m), & \text{if } m \in T_Y \text{ active or not, } T_Y \setminus \{m\} \text{ not active.} \end{cases} \tag{48}$$

*Proof* Variables  $p_l \quad \forall l \in T_Y$  and  $y_l \quad \forall l \in T_Y$  can be substituted out from Problem P–5.12 using the penultimate (quality balances) and second (flow balances) constraint types, respectively. Hence, Problem P–5.12 becomes parametric on  $p_l \quad \forall l \in T_Y$  with optimal objective

$$\max_{\{x_{i,l}\}, \{y_l\}, \{z_i\}, \{p_l\}} f = \max_{\{x_{i,l}\}, \{z_i\}} f(p_1, \dots, p_L). \tag{49}$$

For fixed pool concentrations  $p_l \quad \forall l \in T_Y$ , all pools have fixed optimal cost  $\gamma_l$  (obtained as  $\gamma_l = \gamma_{ij}(p_l)$  with  $\mathcal{A}_I(p_l) = ij$  for I-1-1 instances according to Section 3.1) and thus behave like additional directs sending flow directly to the output. Consequently, Theorem 3.2.9 for directs-only instances from Section 3.2 applies, implying that maximum two nodes among pools and directs are active.

The case with two pools active (see Fig. 9) is treated separately in Eq. (48) as a two pool parametric restriction of Eq. (49) where no directs are active (therefore associated flow variables  $\{z_i\}$  can be eliminated). The second case in Eq. (48) aggregates the cases with maximum one pool active, and corresponds directly to the class of Problems P–3.4 solved in Section 3.3.  $\square$

**Theorem 5.3** (*Solution for two active pools at an input dominance breakpoint*)

The solution of Problem P–5.12 with two active pools  $m, n$  is found at  $(p_m^b, p_n^b)$ , where  $(\forall i \in \{m, n\}) p_i^b$  is an input dominance breakpoint along  $p_i$  in a single  $i$  pool I-1-1 sub-instance (Section 3.1), i.e.:

$$\max_{\{x_{i,m}\}, \{x_{i,n}\}} f(p_m, p_n) = \max_{(p_m^b, p_n^b) \in \mathcal{B}_{I(m)} \times \mathcal{B}_{I(n)}} f^*(p_m^b, p_n^b), \tag{50}$$

where  $\mathcal{B}_{I(r)}$  as in Theorem 3.1.8, Eq. (18a) for  $f^* = \max_{p_r} f^*(p_r) = \max_{\{x_{i,r}\}, \{z_i\}} f(p_r)$ .

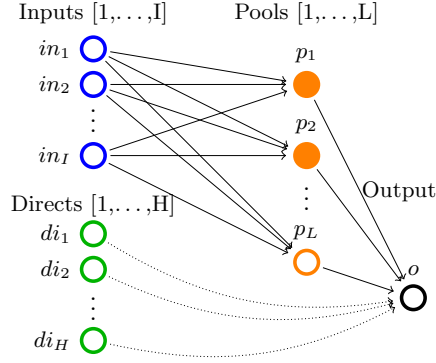


Fig. 9: Two active pools (filled nodes) in an I+H-L-1 instance.

*Proof* Suppose concentration  $p_n$  is fixed which implies pool  $n$  acts as an additional direct with fixed concentration and cost (optimal). Since  $p_m, p_n$  are independent, parametric optimal objective  $f^*(p_m, p_n)$  behaves like  $f^*(p_m)$  in a single  $m$  pool problem where  $n$  acts as a direct, not as a pool. Pools  $m, n$  both active implies that  $\forall p_m$  the dominant active set for  $f^*(p_m)$  is a mixed active set  $\{i, j, n\}$  with  $n$  as a direct and  $\{i, j\}$  the dominant active input set sending flow to  $m$ . Since  $n$  must be active and therefore part of the dominant active set, a change in the dominant active set can only occur with a change of dominant active input set  $\{i, j\}$ , independently of  $n$  and therefore fixed value  $p_n$ . Consequently, the dominance breakpoints of  $f^*(p_m, p_n)$  w.r.t.  $p_m$  occur independently of the value of  $p_n$  and are always breakpoints between dominant active input sets for pool  $m$ . The vice-versa independence also holds. Excluding input dominance breakpoint pairs of  $f^*(p_m, p_n)$  w.r.t both  $p_m, p_n$  in  $\mathcal{B}_{I(m)} \times \mathcal{B}_{I(n)}$ , function  $f^*(p_m, p_n)$  is linear (Lemma 3.1.1) in at least one parameter (with gradient non-zero). Hence, Eq. (50) follows.  $\square$

**Corollary 5.4** (*Strongly-polynomial time complexity*)

Problem P–5.12 is solved in strongly-polynomial worst-case time

$$O\left((I^3 + H^3) \cdot L + I^2 \cdot L^2\right) \quad (51)$$

*Proof* According to Theorems 3.1.8 and 5.3, the first case in Eq. (48) for two given active pools involves  $2 \cdot O(I^3)$  time for finding the two sets of input dominance breakpoints and  $O(I^2)$  for evaluating the optimal parametric objective function at all breakpoint pairs. Since there are  $\binom{L}{2}$  possible pairs of active pools, the total time for the first case of Eq. (48) is  $O(I^3 \cdot L) + O(I^2 \cdot L^2)$ .

The second case in Eq. (48) for one possibly active pool is equivalent to solving Problem P–3.4 (Theorem 3.3.9) and there are  $L$  active pool choices for a total time  $O((I^3 + H^3) \cdot L)$ .

Adding the two cases of Eq. (48) yields the time complexity in Eq. (51).  $\square$

Fig. 10 illustrates the I+H-L-1 instance with a numerical example showcasing the implications of Theorem 5.2 and Theorem 5.3. For a chosen parametrization as in Fig. 10, the parametric function  $f^*(p_1, p_2)$  reveals portions of the domain where only one pool is active (around the edges of the cube) corresponding to the second case in Eq. (48) with piecewise-monotone structure (as shown in Section 3.3). Other portions of the domain (in the neighbourhood of  $p_1 = 2.5, p_2 = 3$ ), however, correspond to the first case in Eq. (48), when both pools are active.

**Remark 5.5** (*Sparsity results extend to a multi-layered network*) Theorem 5.2 extends the sparsity results from the input layer to the pool layer. These sparsity results would also hold for networks with more layers.

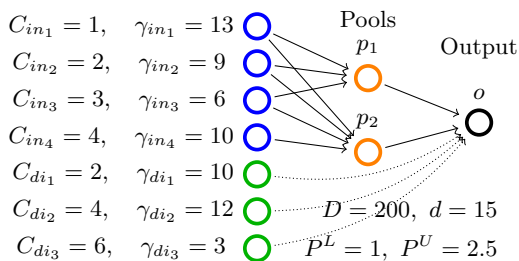
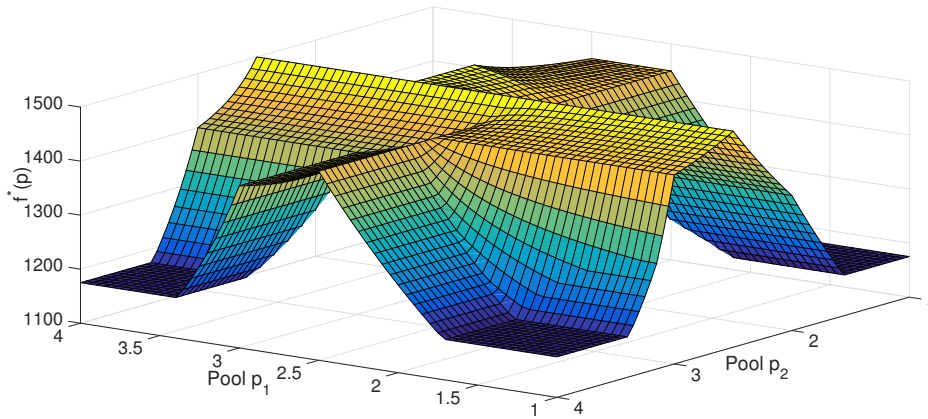


Fig. 10: Parametric optimal objective function  $f^*(p_1, p_2)$  vs. pools concentrations  $p_1, p_2$  for a two-pool, one output network with four inputs and three directs (parametrized with concentrations/costs). The objective is a piecewise-monotone convex/concave/linear function w.r.t.  $p_1$  or  $p_2$  individually.

**Remark 5.6** (Assumptions: Analytical solutions/sparsity/piecewise structure versus LP)

This section finds analytically the optimal solution for a I+H-L-1 pooling topology with Assumption 2.2. Since the I+H-L-1 instance is an LP extension of the I+H-1-1 instance, relaxing any constraint assumption, as described in Remark 3.3.10, will lead to intractable analytical solutions, vanishing sparse structure and having to solve the LP.

## 6 Concluding remarks

This paper builds a framework analyzing standard pooling problem instances by parametrizing the objective function with respect to pool concentrations. The bottom-up analysis develops strongly-polynomial time algorithms for multiple pooling network topological instances, all in the presence of a single quality, an unbounded number of feeds to pools and also outputs (direct bypass flows) and certain flow assumptions. Patterns and hierarchies of dominating topologies are used to find active network structure. The sparsity identified in the active network structure at optimality is then linked to a pool parametric piecewise structure of the objective function. The result reveals analytically Professor Floudas’ intuition of piecewise structure in pooling problem instances.

The parametric objective function is then shown to be piecewise-monotone for instances with one output, allowing exact global solutions in strongly-polynomial time as alternatives to black-box linear programming. The insights are further used for non-linear instances with multiple outputs and one pool to overcome piecewise non-monotonicity via stationary points found in strongly-polynomial time. This result introduces a new reference point on the  $P/NP$  boundary for standard pooling instances, as any relaxation of assumptions or full topology (multiple pools and outputs) are shown to reach NP-hardness. The multiple outputs instance and its assumptions includes the Haverly [32] pooling problems, showing for the first time they have exact, analytical solutions.

The position on the  $P/NP$  boundary of the multiple outputs and one pool instance is thus an ideal starting point for approximating algorithms that cross into NP-hardness. Moreover, this paper developed intuition around sparse solutions and the conditions under which sparsity vanishes. This encourages future research in building disjunctive cuts based on the structures identified to partition feasible space in the non-sparse NP-hard instances, an approach taken by the state-of-the-art heuristic developed in [20].

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## A Omitted Proofs

### Proof of Lemma 3.2.4.i-ii:

(i) Lemma 3.2.2 implies w.l.o.g. that  $C_i > P^U$  (the other case  $C_i < P^L$  is analogous). Then  $C_j < P^U$ , otherwise  $(C_i z_i + C_j z_j)/(z_i + z_j) > P^U$  implying  $\{i, j\}$  infeasible. Two cases now arise:

1.  $C_j > P^L$ : Then  $\gamma_i < \gamma_j$ , otherwise  $j \succeq \{i, j\}$ . Therefore increasing the cheaper flow  $z_i$  maximizes  $f$ , but since  $C_i > C_j$ , doing so also increases concentration  $(C_i z_i + C_j z_j)/(z_i + z_j)$ , which should not exceed  $P^U$  for feasibility. Consequently,  $(C_i z_i + C_j z_j)/(z_i + z_j) = P^U$ .
2.  $C_j < P^L$ : If  $\gamma_i < \gamma_j$  then, as in the previous case,  $(C_i z_i + C_j z_j)/(z_i + z_j) = P^U$ . Otherwise, if  $\gamma_i > \gamma_j$ , decreasing output concentration till bound  $P^L$  and therefore increasing weight of lower cost  $\gamma_j$  maximizes  $f$ , so  $(C_i z_i + C_j z_j)/(z_i + z_j) = P^L$ .

Analogously when  $C_i < P^L$ , if  $P^L < C_j < P^U$  then  $(C_i z_i + C_j z_j)/(z_i + z_j) = P^L$ , or else if  $C_j > P^U$  then  $(C_i z_i + C_j z_j)/(z_i + z_j) = P^L$  or  $P^U$  (depending on whether  $\gamma_i < \gamma_j$  or  $\gamma_i > \gamma_j$ , respectively). Aggregating all the cases analyzed,  $(C_i z_i + C_j z_j)/(z_i + z_j) = P^L$  if  $(C_i - C_j)(\gamma_i - \gamma_j) > 0$  and  $(C_i z_i + C_j z_j)/(z_i + z_j) = P^U$  if  $(C_i - C_j)(\gamma_i - \gamma_j) < 0$ , corresponding to Definition 3.2.3 of  $P(i, j)$ .

(ii) If  $\{i, j\}$  satisfies Item i, due to Lemma 3.2.2 and Lemma 3.2.1.ii assume w.l.o.g.  $C_j < P^U < C_i$  (all other cases are analogous), which implies that  $P(i, j) = P^U$  and  $\gamma_i < \gamma_j$ . Now we add node  $k$  to the pair  $\{i, j\}$  showing case-by-case it either does not improve the objective  $f$  or requires the output concentration to reach  $P(i, j) = P^U$ :

1. If  $C_k < P^U$  and  $\gamma_k > \gamma_j$ : By viewing node pair  $\{j, k\}$  as one joint feasible node  $r$  with cost/concentration a linear combination of the respective properties of  $j, k$ , since  $C_j, C_k < P^U$ , then  $C_r < P^U$ . Since  $i$  is infeasible and  $\gamma_r = (\gamma_j z_j + \gamma_k z_k)/(z_j + z_k) > \gamma_i$ , according to Lemma 3.2.2, then  $\{i, r\} \succeq r$ . The conditions in Item i are therefore met, and the output concentration delivered by  $\{i, j, k\} = \{i, r\}$  is  $P(i, r) = P^U$  since  $(C_i - C_r)(\gamma_i - \gamma_r) < 0$ .
2. If  $C_k < P^U$  and  $\gamma_k < \gamma_j$ :
  - i. If  $\gamma_k < \gamma_i$  and  $C_k > P^L$ : Node  $k$  is cheapest and a feasible solution so  $k \succeq \{i, j, k\}$ .
  - ii. If  $\gamma_k < \gamma_i$  and  $C_k < P^L$ : Node  $k$  is cheapest and infeasible and since  $(C_i - C_k)(\gamma_i - \gamma_k) > 0$  we have  $P(i, k) = P^L$ . Thus  $\{i, k\} \succeq \{i, j, k\}$  since  $\gamma_j > \gamma_i > \gamma_k$ .
  - iii. If  $\gamma_k > \gamma_i$ : We have  $\gamma_j > \gamma_k > \gamma_i$  and we are in case 1 with indices  $j, k$  swapped.
3. If  $C_k > P^U$  and  $\gamma_k < \gamma_i$ : Same argument as in case 1 applies, viewing pair  $\{i, k\}$  as one joint node  $r$ . The exception is that now pair  $\{i, k\}$  is infeasible with  $C_r > P^U$  and can not therefore dominate triple  $\{i, j, k\}$ . Since  $(C_j - C_r)(\gamma_j - \gamma_r) < 0$ , then  $P(j, r) = P^U$ .
4. If  $C_k > P^U$  and  $\gamma_k > \gamma_i$ :
  - i. If  $\gamma_k > \gamma_j$ : Then  $\{i, j\} \succeq \{i, j, k\}$  since node  $k$  is the most expensive and infeasible.
  - ii. If  $\gamma_k < \gamma_j$ : Then  $\gamma_j > \gamma_i > \gamma_k$  and we are in case 3 with indices  $i, k$  swapped.

□

**Proof of Lemma 3.2.8.i:**

Let  $P = \{i, j\}$ ,  $T = \{i, j, k\}$ . If the triple  $T$  is trivially dominated by a subset, then if it is dominated by a pair or node  $i$  or  $j$ , since  $\{i, j\}$  dominates all pairs and both its individual nodes, by transitivity  $T$  is dominated by  $\{i, j\}$ . If  $T$  is not dominated by a subset pair or node  $i$  or  $j$  but only by node  $k$ , it means  $C_k \in [P_L, P_U]$  and  $k \succeq T \succeq \{i, k\}, \{j, k\}$ . Therefore  $\gamma_k < \gamma_i, \gamma_j$ . But the pair formed by  $k$  and the node among  $i, j$  with the lower cost would dominate  $T$ , contradiction. So  $T$  is always dominated by a pair subset or node  $i$  or  $j$ , meaning  $\{i, j\}$  always dominates  $T$  by transitivity.

If  $T$  is not trivially dominated by a subset, due to Item ii, we have  $(C_i z'_i + C_j z'_j + C_k z'_k) / (z'_i + z'_j + z'_k) = P(i, j)$  (prime notation of flows to distinguish them from flows associated to active pair  $\{i, j\}$ ). The optimal costs (optimality \* superscript omitted for simplicity) used to establish dominance in Eq. (2) between  $P$  and  $T$  are,

$$\begin{cases} h_P = \gamma_i z_i + \gamma_j z_j, & \text{with } P(i, j) = \frac{C_i z_i + C_j z_j}{z_i + z_j}, & D = z_i + z_j, \\ h_T = \gamma_i z'_i + \gamma_j z'_j + \gamma_k z'_k, & \text{with } P(i, j) = \frac{C_i z'_i + C_j z'_j + C_k z'_k}{z'_i + z'_j + z'_k}, & D = z'_i + z'_j + z'_k. \end{cases}$$

Substituting  $z_i, z_j$  from Eq. (20) in  $h_P$  we have  $h_P = \frac{D(\gamma_i(P(i, j) - C_j) - \gamma_j(P(i, j) - C_i))}{C_i - C_j}$ . Solving similarly for  $z'_i, z'_j$  in terms of  $z'_k$  from the equations above leads to:

$$z'_i = \frac{D(P(i, j) - C_j) - z'_k(C_k - C_j)}{C_i - C_j}, \quad z'_j = \frac{-D(P(i, j) - C_i) + z'_k(C_k - C_i)}{C_i - C_j}.$$

Introducing the above formulas for  $z'_i, z'_j$  into  $h_T$  and subtracting  $h_P$ , the following condition for  $P \succeq T$  results:

$$\begin{aligned} h_T - h_P &= \gamma_k z'_k + z'_k \left( \gamma_j \frac{C_k - C_i}{C_i - C_j} - \gamma_i \frac{C_k - C_j}{C_i - C_j} \right) \\ &= z'_k \frac{C_k(\gamma_j - \gamma_i) + C_i(\gamma_k - \gamma_j) + C_j(\gamma_i - \gamma_k)}{C_i - C_j} > 0. \end{aligned} \quad (52)$$

If  $(C_i - C_j)(C_k - C_j) < 0$ , then  $C_j$  is between  $C_i$  and  $C_k$ , and thus  $(C_j - C_i)(C_k - C_i) > 0$ . Therefore  $\exists \alpha \in \{i, j\}$  s.t.  $(C_\beta - C_\alpha)(C_k - C_\alpha) > 0$ ,  $\beta \in \{i, j\} \neq \alpha$  and if w.l.o.g.  $\alpha = j$  then  $(C_i - C_j)(C_k - C_j) > 0$ . Since  $\{i, j\}$  dominates any other pair, then  $\{i, j\} \succeq \{k, j\}$  and comparing the two pairs using Eq. (21a) results in:

$$\begin{aligned} P(i, j) \left( \frac{\gamma_i - \gamma_j}{C_i - C_j} \right) + \frac{\gamma_j C_i - \gamma_i C_j}{C_i - C_j} &< P(k, j) \left( \frac{\gamma_k - \gamma_j}{C_k - C_j} \right) + \frac{\gamma_j C_k - \gamma_k C_j}{C_k - C_j} \\ \Leftrightarrow \frac{(C_j - P(i, j))(C_k(\gamma_j - \gamma_i) + C_i(\gamma_k - \gamma_j) + C_j(\gamma_i - \gamma_k))}{(C_i - C_j)(C_k - C_j)} &- (P(k, j) - P(i, j)) \left( \frac{\gamma_k - \gamma_j}{C_k - C_j} \right) < 0. \end{aligned} \quad (53)$$

Since if  $(\gamma_k - \gamma_j)/(C_k - C_j) > 0$  then  $P(k, j) - P(i, j) = P^U - P(i, j) \geq 0$  and otherwise  $P(k, j) - P(i, j) = P^L - P(i, j) \leq 0$ , we have that  $(P(k, j) - P(i, j))(\gamma_k - \gamma_j)/(C_k - C_j) \geq 0$ . This implies from Eq. (53) that:

$$\frac{(C_j - P(i, j))(C_k(\gamma_j - \gamma_i) + C_i(\gamma_k - \gamma_j) + C_j(\gamma_i - \gamma_k))}{(C_i - C_j)(C_k - C_j)} < 0 \quad (54)$$

The conditions in Eq. (52) and Eq. (54) are equivalent due to the fact that  $(C_i - C_j)(C_k - C_j)$  and  $z'_k$  are always positive,  $C_j - P(i, j)$  has the same sign of  $C_j - C_i$  (since  $P(i, j)$  must be in-between  $C_j, C_i$ ), and the remaining factor is identical. Therefore,  $\{i, j\} \succeq \{k, j\} \Leftrightarrow$  Eq. (54)  $\Leftrightarrow$  Eq. (52)  $\Leftrightarrow P = \{i, j\} \succeq \{i, j, k\} = T$ .  $\square$



**Proof of Lemma 3.3.3:**

For Problem P-3.4,  $f_{ij} = dD - x_i\gamma_i - x_j\gamma_j$  and  $f_{\{ij,q\}} = dD - x'_i\gamma_i - x'_j\gamma_j - z_q\gamma_q$ . Therefore,

$$ij \preceq_p \{ij, q\} \Leftrightarrow x_i\gamma_i + x_j\gamma_j \geq x'_i\gamma_i + x'_j\gamma_j + z_q\gamma_q,$$

which, by replacing all flows with their solutions from Eq. (7) and Eq. (23), can be rewritten as:

$$\gamma_{ij}(p) \geq \gamma_{\{ij,q\}}(p) \Leftrightarrow \frac{D(p - P(ij, q))(\gamma_i(p - C_j) + \gamma_j(C_i - p) + \gamma_q(C_j - C_i))}{(C_i - C_j)(p - C_q)} \geq 0.$$

Since constant demand  $D > 0$  and output concentration  $P(ij, q)$  is a linear combination of  $p, C_q$ , then  $D(p - P(ij, q))/(p - C_q) \geq 0$  and the dominance condition becomes:

$$\frac{\gamma_i(p - C_j) + \gamma_j(C_i - p) + \gamma_q(C_j - C_i)}{C_i - C_j} \geq 0 \Leftrightarrow \gamma_{ij} = \frac{\gamma_i(p - C_j) + \gamma_j(C_i - p)}{C_i - C_j} \geq \gamma_q.$$

with the breakpoint achieved by solving for  $p$  at equality.  $\square$

**Proof of Proposition 3.3.5.ii:**

For any breakpoint  $p$  between  $\{i, j, q\}$  and  $\{i, j, r\}$ , the following must hold,

$$\{i, j, q\} \succ_p \{i, j, r\} \stackrel{\text{Eq. (3)}}{\Leftrightarrow} \gamma_i x_i + \gamma_j x_j + \gamma_q z_q = \gamma_i x'_i + \gamma_j x'_j + \gamma_r z_r,$$

which after replacing the flow variables on both sides from Eq. (23), becomes,

$$\begin{aligned} & \frac{\gamma_i(p - C_j)(P(ij, q) - C_q)}{(C_i - C_j)(p - C_q)} + \frac{\gamma_j(p - C_i)(P(ij, q) - C_q)}{(C_j - C_i)(p - C_q)} + \frac{\gamma_q(p - P(ij, q))}{p - C_q} = \\ & \frac{\gamma_i(p - C_j)(P(ij, r) - C_r)}{(C_i - C_j)(p - C_r)} + \frac{\gamma_j(p - C_i)(P(ij, r) - C_r)}{(C_j - C_i)(p - C_r)} + \frac{\gamma_r(p - P(ij, r))}{p - C_r}. \end{aligned}$$

Multiplying out the common denominator of all terms and then grouping the first two terms from each side and factoring out  $p$  results in:

$$\begin{aligned} & p^2(\gamma_i - \gamma_j)((P(ij, q) - C_q) - (P(ij, r) - C_r)) \\ & + p \left( (P(ij, r)C_q - P(ij, q)C_r)(\gamma_i - \gamma_j) - (\gamma_i C_j - \gamma_j C_i)((P(ij, q) - C_q) - (P(ij, r) - C_r)) \right) \\ & - (\gamma_i C_j - \gamma_j C_i)(P(ij, r)C_q - P(ij, q)C_r) \\ & + p^2(C_i - C_j)(\gamma_q - \gamma_r) + p(C_i - C_j)(\gamma_r C_q + \gamma_r P(ij, r) - \gamma_q C_r - \gamma_q P(ij, q)) \\ & + (C_i - C_j)(\gamma_q C_r P(ij, q) - \gamma_r C_q P(ij, r)) = 0. \end{aligned}$$

Assuming  $P(ij, q)$  and  $P(ij, r)$  are independent of  $p$  results in a quadratic equation in terms of  $p$ ,

$$\Gamma(p, P(ij, q), P(ij, r)) = p^2(a_1 b_1 + a_3 c_1) + p(a_1 b_2 - a_2 b_1 + a_3 c_2) + (a_3 c_3 - a_2 b_2) = 0,$$

with the following notation:

$$\begin{aligned} a_1 &= \gamma_i - \gamma_j, & b_1 &= (P(ij, q) - C_q) & c_1 &= \gamma_q - \gamma_r, \\ a_2 &= \gamma_i C_j - \gamma_j C_i, & & (P(ij, r) - C_r), & c_2 &= \gamma_r(C_q + P(ij, r)) - \gamma_q(C_r + P(ij, q)), \\ a_3 &= C_i - C_j, & b_2 &= P(ij, r)C_q - P(ij, q)C_r, & c_3 &= \gamma_q C_r P(ij, q) - \gamma_r C_q P(ij, r). \end{aligned}$$

Assuming  $\Delta^2 > 0$ ,  $\Gamma$  has up to two roots as possible breakpoints,

$$p_{1,2} = \frac{-(a_1 b_2 - a_2 b_1 + a_3 c_2) \pm \sqrt{(a_1 b_2 - a_2 b_1 + a_3 c_2)^2 - 4(a_1 b_1 - a_3 c_1)b_2(a_3 c_3 - a_2 b_2)}}{2(a_1 b_1 - a_3 c_1)}.$$



□

**Proof of Proposition 3.3.7:**

The first constraint of Problem P–3.4 implies  $z_q = D - x_i - x_j$ , which in turn implies,

$$\begin{aligned}
 f_A(p) &= d \cdot D - \gamma_i x_i - \gamma_j x_j - \gamma_q x_q = (d - \gamma_q)D - (\gamma_i - \gamma_q)x_i - (\gamma_j - \gamma_q)x_j, \\
 \frac{\partial f_A}{\partial p} &= \frac{\partial}{\partial p} ((\gamma_i - \gamma_q)x_i + (\gamma_j - \gamma_q)x_j) \\
 &\stackrel{\text{Eq. (23)}}{=} \frac{D(P(ij, q) - C_q)}{C_i - C_j} \cdot \frac{\partial}{\partial p} \left( \frac{(\gamma_i - \gamma_q)(p - C_j)}{p - C_q} - \frac{(\gamma_j - \gamma_q)(p - C_i)}{p - C_q} \right) \\
 &= \frac{D(P(ij, q) - C_q)}{C_i - C_j} \cdot \left( \frac{\partial}{\partial p} \frac{p(\gamma_i - \gamma_j)}{p - C_q} + \frac{\partial}{\partial p} \frac{C_i(\gamma_j - \gamma_q) - C_j(\gamma_i - \gamma_q)}{p - C_q} \right) \\
 &= \frac{D(P(ij, q) - C_q)}{C_i - C_j} \cdot \frac{C_j(\gamma_i - \gamma_q) + C_i(\gamma_q - \gamma_j) + C_q(\gamma_j - \gamma_i)}{(p - C_q)^2} \\
 &= - \frac{D(P(ij, q) - C_q)}{(C_i - C_j)(p - C_q)^2} \cdot \left( C_q(\gamma_j - \gamma_i) + C_j(\gamma_i - \gamma_q) + C_i(\gamma_q - \gamma_j) \right).
 \end{aligned}$$

By deriving to further orders and due to  $\frac{\partial^2 f_A}{\partial p^2} = \frac{-2}{(p - C_q)} \frac{\partial f_A}{\partial p}$ , the desired assertions are obtained. □

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