Application of Primal-Dual Iteration to the Solution of Process Network Synthesis Problems

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Abstract:

The Infinite DimEnsionAl State-space (IDEAS) conceptual framework has been previously applied to various process synthesis problems, including reactor networks [1], reactive distillation networks [2], multi-component mass exchange networks [3], membrane networks [4], power cycle synthesis [5], and distillation networks [6,7]. The IDEAS framework possesses two unique characteristics: it considers all feasible networks and it leads to a convex (linear) optimization formulation.

The IDEAS framework decomposes process networks into two subnetworks: an operator (OP) subnetwork, where process technologies (unit operations) and / or their aggregate effects are represented, and a distribution (DN) subnetwork, where mixing, splitting, recycling, and bypassing operations occur. The OP and DN subnetworks have an infinite number of inlets and outlets, which gives rise to infinite dimensional solutions with a linear feasible region.

The infinite dimensional linear program formulated with the IDEAS framework usually can not be solved explicitly, but rather its solution can be approximated with a series of finite linear programs of increasing size, whose sequence of values converges to the optimum value of the infinite dimensional problem. The size of the finite problem is typically increased with uniform discretization to approximate the condition space of the process operator (space of intensive stream conditions: temperature, pressure, concentration, residence time, etc.), which brings along a significant increase in computational memory requirement.

In this work we consider the possible use of duality theory for the solution of IDEAS-derived infinite linear programs. The motivation is to reduce the computational memory requirements for the finite approximation to the solution of the IDEAS problem.

Problem Statement:

A general equality constrained ILP can be posed in the following form:

$$(1) \qquad \nu = \inf_{x} \left\{ \langle x, c \rangle : Ax = b, \quad x \in X^{+} \right\}$$

Where X^+ is the positive cone of a normed, linear vector space and $A : X \rightarrow Y$ is a linear operator.

Hernandez-Lerma and Lasserre [8] give a set of criteria to prove whether such an ILP is solvable (has a feasible solution x^* that achieves the optimal value v) by successive finite approximations; it must have a non-empty feasible set, have a feasible solution x^0 with $\langle x^0, c \rangle > 0$, and this x^0 must define a set X^0 that is weakly sequentially compact, where X^0 is defined as:

$$(2) \qquad X^0 := \left\{ x \in X^+ \mid \left\langle x, c \right\rangle \leq \left\langle x_0, c \right\rangle \right\}$$

If these conditions are satisfied, problem (1) has an optimal solution x^* and there is no duality gap between the optimal solution to the primal problem and the optimal solution of the dual.

In the IDEAS formulation, the spaces X and Y are considered to be ℓ_1, the space of sequences with a finite absolute sum of elements and the operator A has been shown to be continuous and bounded [9]. A problem of this form is typically solved through solution of successively larger finite dimensional problems which converge to the optimal value of the infinite problem. This method could potentially be improved (in terms of computation time and algorithm efficiency) by incorporating the dual of the primal problem (1) into the finite approximations to find a lower bound on the value of the optimal solution to the infinite problem.

We consider in this work the isothermal, isobaric, constant density, minimum total reactor volume problem within the IDEAS framework. This problem can be formed as follows (for simplicity and without loss of generality we consider only one species):

$$(3) \qquad \nu = \inf_F \left\{ \left\langle F, \tau \right\rangle : Ax = b, \quad F \in \ell_1^+ \right\}$$

where τ and F are sequences defined as follows:

$$(4) \qquad \tau = \left\{ \tau_{ij} \right\}_{i=0, j=0}^{\infty, \infty}$$

$$(\mathit{Where}\ \tau_{ij} \ = \ \tau_i \quad \forall i = 0 \ldots \infty \quad \forall j = 0 \ldots \infty, \quad \tau_0 = 0)$$

$$(5) \qquad F = \left\{ F_{ij} \right\}_{i=0, j=0}^{\infty, \infty}$$

The linear operator A and the sequence b can be constructed from the following set of equalities:

$$(6) \qquad F_0 - \sum_{j=0}^{\infty} F_{j0} = 0$$

$$(7) \qquad \sum_{j=0}^{\infty} \left[\left(C_0^{'} - C_j \right) F_{0j} \right] = 0$$

$$(8) \qquad \sum_{j=0}^{\infty} \left[F_{ij} - F_{ji} \right] = 0 \qquad \forall i = 1 \ldots \infty$$

$$(9) \qquad \sum_{j=0}^{\infty} \left[\left(C_i^{'} - C_j \right) F_{ij} \right] = 0 \qquad \forall i = 1 \ldots \infty$$

Where the variables and parameters are defined as follows:

Variables:

F_0 = Total flow to the network

F_{i0} = Flow from the network inlet to reactor i

F_{0j} = Flow from reactor j to the network outlet

F_{ij} = Flows from the outlet of reactor j to the inlet of reactor i

Parameters:

$C_0^{'}$ = Concentration of reactant in the network outlet

C_0 = Concentration of reactant in the network inlet

$C_i^{'}$ = Concentration of reactant in the feed to reactor i

C_j = Concentration of reactant in the outlet from reactor j

τ_i = Residence time of the i$^{\text{th}}$ reactor = Volume of reactor i / Flow through reactor i

Equation (6) represents a total mass balance on the splitting of the network inlet stream. Equation (7) is a component balance on the mixing of all the streams that add up to the network outlet. Equations (8) define total mass balances on each reactor (total flow in = total flow out). Equations (9) define component balances on the mixing of all the streams that add up to the inlet to each reactor i.

The variable x, which is made up of the flows in the network, is required to be non-negative and to belong to ℓ_1. This restricts the total flow going through all the reactors to be finite. The residence times are also restricted to be non-negative by physical arguments, and are readily identifiable once the values for the inlet and outlet concentrations to each reactor are set.

Problem (1) has a dual of the following form:

$$(10) \qquad v^* = \sup_y \left\{ \langle b, y \rangle : A^T y \le \tau, \quad y \in \ell_\infty \right\}$$

Where b and c are defined as above, A^T is the adjoint of the operator A above and y is the dual variable which belongs to ℓ_∞ (the dual of ℓ_1) i.e. it is a sequence whose values are unrestricted other than that each member of the sequence y is finite. This dual can be represented by the following equivalent formulation:

$$(11) \qquad v^* = \sup_y F_0 y_0$$

$$s.t. \quad y_{2j} - y_1 \left(C_0^{'} - C_j \right) \le 0 \qquad \forall j = 1 \ldots \infty$$

$$y_{2j} - y_{2i} - y_{2i+1} \left(C_i^{'} - C_j \right) \le \tau_i \qquad \forall j = 0 \ldots \infty \quad \forall i = 1 \ldots \infty$$

This problem has some very interesting characteristics; firstly, the objective function depends only on one variable, y_0, which corresponds to the first constraint in the primal problem (equation (4)). Also, while there are an infinite number of variables and constraints in the dual, each constraint has only a finite number of variables in it.

Properties of ILPs (1) and (11) are discussed and their suitability for the creation of an iterative primal-dual scheme for the solution of (1) will be considered.

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