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Mathematical programming (optimization)

Global optimization of water networks design using multiparametric disaggregation

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ABSTRACT

We propose new mixed-integer linear programming models for the optimal design of water-using and wastewater treatment networks. These replace the original non-convex, nonlinear problems following parameterization of the concentration variables appearing in the bilinear terms resulting from the contaminant mass balances. The difference between the models lies in the numeric system used for the parameterization. We show how to perform the transformation for a generic coding and give the results for the decimal and binary systems. While the resulting MILPs are approximations of the original NLP, any desired accuracy level can be set, being the proposed models exact in the limit of an infinite number of significant digits. Through the solution of several test cases taken from the literature, we show that the value of the objective function rapidly approaches the global optimal solution. The models can also be used to initialize the NLP when solved with local optimization solvers.

1. Introduction

Many nonlinear programming (NLP) problems of practical interest in chemical engineering involve bilinear terms of continuous variables resulting from the material balance equations for multicomponent streams (Quesada & Grossmann, 1995), where each stream is associated with a flow and a set of properties. Well-known examples include process networks (Ruiz & Grossmann, 2011), pooling (Gounaris, Misener, & Floudas, 2009) and water network design (Jezowski, 2010). Such bilinear programs are nonconvex, giving rise to multiple local optima and making the application of local NLP solvers ineffective, either due to a suboptimal solution outcome or even failure to locate a feasible one. Since the objective function is typically related to an economic metric, guaranteeing global optimality is of major importance.

The most common global optimization algorithms are based on spatial branch and bound (Wicaksono & Karimi, 2008) and have in common the relaxation of the bilinear terms with the McCormick (1976) linear envelope, which represents the tightest possible convex relaxation (Al-Khayyal & Falk, 1983). Branch and bound methods work by approaching an upper bound (UB), generated from the solution of the original NLP problem with a local solver (when minimizing), to a lower bound (LB), calculated from the solution of the relaxed linear program (LP), within a given tolerance ε. The relaxation becomes increasingly tighter by reducing the domain of the variable(s) selected for branching, which can be both discrete and continuous. A commercial application of a spatial branch and bound algorithm featuring the standard McCormick relaxations for the bilinear terms is the branch and reduce global optimization solver BARON (Sahinidis, 1996; Tawarmalani & Sahinidis, 2002).

One interesting aspect of mathematical programming is that a few alternatives typically exist to formulate a problem, as can be seen in the CMU-IBM Cyber-Infrastructure for MINLP collaborative site (http://minlp.org/). In the case of bilinear programs, the type and number of variables involved in the nonconvex terms can have an important impact on the quality of the relaxation. Liberti and Pantelides (2006) have proposed an algorithm that may sometimes provide useful insights on how best to formulate a bilinear program. It transforms the original problem into an equivalent one with fewer bilinear terms, with the resulting formulation featuring additional linear constraints that do not affect the feasible region of the original NLP but tighten that of its convex relaxation. While limited to linear equality constraints, their algorithm is more selective at identifying multiplications that result in valid sets of constraints when compared to the original reformulation linearization technique (RLT) of Sherali and Alameddine (1992). Quesada and Grossmann (1995) also used some ideas of RLT to establish a relation between formulations based on compositions and individual flows for the case of process network problems. For this class of problems, Ruiz and Grossmann (2011) have recently exploited the interaction between the vector spaces of

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Nomenclature

Sets/indices/superscripts

C, c process contaminants
D, d wastewater streams
E, e environment
J, j possible values in any given position of the numeric system representation
K, k positions in the numeric system representation
K_{bin} positions in the binary system representation
K_{dec} positions in the decimal system representation
T, t, t' wastewater treatment units
U, u, u' water-using units
U^{ff} fixed flowrate units
U^{fl} fixed load units
W, w freshwater streams

Parameters

$c^{D}_{d,c}$ concentration of contaminant c in wastewater stream d
$\bar{c}^{E}_{c}$ maximum environmental discharge concentration for contaminant c
$\bar{c}^{U\text{-}in}_{u,c}$ maximum inlet concentration of contaminant c to water-using unit u
$\bar{c}^{U\text{-}out}_{u,c}$ maximum outlet concentration of contaminant c from water-using unit u
$\bar{c}^{T\text{-}in}_{t,c}$ maximum inlet concentration of contaminant c to treatment unit t
$c^{W}_{w,c}$ concentration of contaminant c in freshwater source w
f^{D}_{d} inlet flowrate of wastewater stream d to WTN system
f^{E} inlet flowrate to WTN system, which is equal to final discharge flowrate
$f^{U\text{-}in}_{u}$ inlet flowrate to fixed flowrate unit u
$f^{U\text{-}lim}_{u}$ limiting flowrate of fixed load unit u
$f^{U\text{-}out}_{u}$ outlet flowrate from fixed flowrate unit u
$rr_{t,c}$ removal ratio for contaminant c in treatment unit t
$\Delta m^{U}_{u,c}$ mass of contaminant c entering the system through fixed load unit u
η left truncating point when approximating the parameterized variables (decimal representation)
φ multiplication factor for WTN system
ψ right truncating point when approximating the parameterized variables (decimal representation)

Operator

$\Phi(k,\psi)$ multiplication factor for disaggregated variables for position k of chosen numeric representation system and approximation setting ψ

Variables

$C^{T\text{-}in}_{t,c}$ inlet concentration to treatment unit t for contaminant c (ppm)
$C^{T\text{-}out}_{t,c}$ outlet concentration from treatment unit t for contaminant c (ppm)
$C^{U\text{-}in}_{u,c}$ inlet concentration to fixed-load unit u for contaminant c (ppm)
$C^{U\text{-}out}_{u,c}$ outlet concentration from fixed-load unit u for contaminant c (ppm)
$F^{D\text{-}E}_{d}$ flowrate of wastewater stream d from WUN system bypassing the treatment system into the final discharge mixer (ton/h)
$F^{D\text{-}T}_{d,t}$ flowrate of wastewater stream d from WUN system into treatment unit t (ton/h)
F^{T}_{t} flowrate through treatment unit t (inlet = outlet) (ton/h)
$F^{T\text{-}E}_{t}$ outlet flowrate from treatment unit t going to the final discharge mixer (ton/h)
$\widehat{F}^{T-E}_{t,c,j,k}$ disaggregated flowrate variable linked to $F^{T\text{-}E}_{t}$, contaminant c and value j in position k (ton/h)
$F^{T\text{-}T}_{t',t}$ outlet flowrate from treatment unit t' going to treatment unit t (ton/h)
$\widehat{F}^{T\text{-}T}_{t',t,c,j,k}$ disaggregated flowrate variable linked to $F^{T\text{-}T}_{t',t}$, contaminant c and value j in position k (ton/h)
F^{U}_{u} flowrate through water-using unit u (inlet = outlet) (ton/h)
F^{U-D}_{u} outlet flowrate from water-using u going to the WTN system (ton/h)
$\widehat{F}^{U\text{-}D}_{u,c,j,k}$ disaggregated flowrate variable linked to $F^{U\text{-}D}_{u}$, contaminant c and value j in position k (ton/h)
$F^{U\text{-}U}_{u',u}$ outlet flowrate from water-using unit u' going to water-using unit u (ton/h)
$\widehat{F}^{U\text{-}U}_{u',u,c,j,k}$ disaggregated flowrate variable linked to $F^{U\text{-}U}_{u',u}$, contaminant c and value j in position k (ton/h)
$F^{W\text{-}U}_{w,u}$ flowrate from freshwater w into water-using unit u (ton/h)
$M^{T\text{-}in}_{t,c}$ inlet mass flow of contaminant c to treatment unit t (g/h)
$M^{T\text{-}out}_{t,c}$ outlet mass flow of contaminant c from treatment unit t (g/h)
$M^{U-in}_{u,c}$ inlet mass flow of contaminant c to water-using unit u (g/h)
$M^{U\text{-}out}_{u,c}$ outlet mass flow of contaminant c from water-using unit u (g/h)
$Y^{U}_{u,c,j,k}$ binary variable indicating that value j in position k is active for contaminant c in water-using unit u
$Y^{T}_{t,c,j,k}$ binary variable indicating that value j in position k is active for contaminant c in treatment unit t

properties, flows and the unit vector, in order to generate cuts that are not dominated by McCormick envelopes and will thus tighten the relaxation. However, no theoretical and/or systematic framework exists to date for deriving RLT formulations with predictably efficient performance for general non-convex programs (Wicaksono & Karimi, 2008). These redundant constraint methods can be viewed as a preliminary stage in spatial branch and bound algorithms.

McCormick relaxations can be very week or loose, and may be very slow in lifting the lower bound in a global optimization algorithm. In particular, Androulakis, Maranas, and Floudas (1995) have showed that the maximum difference between the relaxed and real value of a bilinear term is proportional to the area of the domain under consideration. As a remedy, recent works have been exploring the idea of piecewise mixed integer linear programming (MILP) relaxation, still based on the convex envelope of the bilinear term, to some success. Bergamini, Aguirre, and Grossmann (2005) proposed an outer approximation deterministic algorithm for process networks. Meyer and Floudas (2006) have shown that a piecewise linear RLT formulation achieves considerably tighter bounds when compared to the standard convex envelope and an improved RLT formulation, for an industrial case study comprising a generalized pooling problem. Karuppiah and Grossmann (2006) applied the piecewise under- and overestimators under a spatial branch and contract algorithm for the synthesis of an integrated water system.