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A review of recent advances in global optimization

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Abstract This paper presents an overview of the research progress in deterministic global optimization during the last decade (1998–2008). It covers the areas of twice continuously differentiable nonlinear optimization, mixed-integer nonlinear optimization, optimization with differential-algebraic models, semi-infinite programming, optimization with grey box/nonfactorable models, and bilevel nonlinear optimization.

Keywords Global optimization · NLP · MINLP · DAE · SIP · Nonfactorable models · Bilevel optimization

1 Introduction

Global optimization addresses the computation and characterization of global solutions to nonconvex continuous, mixed-integer, differential-algebraic, bilevel, and non-factorable problems. Given an objective function f that is to be minimized and a set of equality and inequality constraints S, the main task of *Deterministic Global Optimization* is to determine (with theoretical guarantees) an epsilon global minimum of the objective function f subject to the set of constraints S. Besides this, global optimization focuses also on the important issues of how to determine lower and upper bounds on the global minimum of the objective function f that are valid for the whole feasible region S, and how to determine an ensemble of good quality local solutions in the vicinity of the global solution. Other objectives may involve the enclosure of all solutions of a set of equality and inequality constraints S, or proving that a constrained nonlinear problem is feasible or infeasible.

Global optimization has found an increased number of applications not only in Chemical Engineering but also across all branches of engineering, applied sciences, and sciences. Complex problems, like the ones arising in refinery pooling, azeotropic distillation and phase and chemical equilibrium, have been tackled by global optimization approaches. Furthermore,

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many interesting mathematical problems, such as the enclosure of all solutions of systems of nonlinear equations or the parameter estimation in nonlinear algebraic models, can be expressed with global optimization formulations.

During the last decade, 1998–2008, several outstanding textbooks have been published addressing different facets of global optimization. These include the textbooks by Tuy (1998) on convex analysis, Bard (1998) on bilevel programming, Sherali and Adams (1999) on the reformulation–linearization technique (RLT), Horst et al. (2000), Floudas (2000a) and Horst and Tuy (2003) on deterministic approaches, Rubinov (2000) on abstract convexity, Strongin and Sergeyev (2000) on sequential and parallel algorithms, Tawarmalani and Sahinidis (2002a) on modeling and implementation issues, Zabinsky (2003) and Zhigljavsky and Zilinskas (2007) on stochastic approaches, Hansen and Walster (2004) on interval methods, and Price et al. (2005) on differential evolution algorithms.

Collection of essays in the area of global optimization were edited by Hadjisavvas and Pardalos (2001), Pardalos and Romeijn (2002), and Audet et al. (2005). In addition to the above, many collections of contributed papers were also published. These include the books by Floudas and Pardalos (2000) that covers advances in the areas of computational chemistry and molecular biology, Migdalas et al. (2001), Dzemyda et al. (2002) that focuses on stochastic methods, Floudas and Pardalos (2003), Liberti and Maculan (2006) that includes implementation discussions and commercial software presentation, as well as by Törn and Zilinskas (2007) on global optimization algorithms of various kinds. An essay on parallel computing in global optimization was presented by D'Apuzzo et al. (2006).

The last decade saw also the launch of the Encyclopedia of Optimization (Floudas and Pardalos 2001), an effort to systematically compile results in the field and present them in an orderly and carefully designed fashion. Providing extensive references for each entry, the Encyclopedia introduces the reader to a complete set of topics that show the spectrum of research, the richness of ideas, and the breadth of applications that has come from the field of Optimization. The effort has experienced wide success and a revised edition appeared recently (Floudas and Pardalos 2008).

The introduction of many algorithms and the need for their computational comparison led to the development of standardized collections of benchmark problems. Such collections of problems in local and global optimization can be found in the handbook by Floudas et al. (1999), the benchmark suite compiled by Shcherbina et al. (2003), as well as in other publications (Casado et al. (2003); Ali et al. (2005)). The benchmark suite was used by Neumaier et al. (2005) to perform a computational comparison between eight global optimization solvers with the help of the COCONUT environment (Schichl 2004).

Finally, a number of review papers discussed the various advances in the field. Floudas (2000b) presented a review on global optimization in the design and control of chemical process systems, while Pardalos et al. (2000) presented advances and research trends on deterministic and stochastic global optimization during the nineties. A survey paper by Neumaier (2004) discussed constrained global optimization and continuous constraint satisfaction problems with a particular emphasis on the use of complete techniques that provably find all solutions. More recently, Floudas et al. (2005) provided a thorough review of developments that covered the years 1998–2003.

In this paper, we will discuss the deterministic global optimization advances during the last ten years (1998–2008) for the following classes of mathematical problems: (i) twice continuously differentiable nonlinear optimization, NLPs; (ii) mixed-integer nonlinear optimization, MINLPs; (iii) differential-algebraic systems, DAEs; (iv) semi-infinite programming, SIP; (v) grey-box and nonfactorable problems; and (vi) bilevel nonlinear optimization.

2 Twice continuously differentiable NLPs

In the first part of this section, we will review the advances in convex envelopes and underestimators, convexification techniques for twice continuously differentiable NLPs, and results regarding concave, bilinear and fractional models. We will subsequently cover other theoretical and algorithmic advances in the area of C^2 NLPs, including results that are focused on particular applications. Finally, we will focus on advances for the global optimization of phase equilibrium and parameter estimation problems.

2.1 Convex envelopes

Tawarmalani and Sahinidis (2001) developed the convex and concave envelopes for x/y over a unit hypercube, compared it to the convex relaxation proposed by Zamora and Grossmann (1998a,b, 1999), proposed a semidefinite relaxation of x/y, and suggested convex envelopes for functions of the form $f(x)y^2$ and $f(x)/y$. Liberti and Pantelides (2003) proposed a nonlinear continuous and differentiable convex envelope for monomials of odd degree, derived its linear relaxation, and compared their results with other relaxation methods.

Meyer and Floudas (2003) studied trilinear monomials with positive or negative domains, derived explicit expressions for the facets of the convex and concave envelopes and showed that these outperform the previously proposed relaxations based on arithmetic intervals or recursive arithmetic intervals. In a later publication (Meyer and Floudas 2004), they presented the results for the case of mixed-sign domains.

Tardella (2003) studied the class of functions whose convex envelope on a polyhedron coincides with the convex envelope based on the polyhedron vertices, and proved important conditions for a vertex polyhedral convex envelope. Meyer and Floudas (2005a) described the structure of the polyhedral convex envelopes of edge-concave functions over polyhedral domains using geometric arguments. They developed an algorithm for computing the facets of the convex envelope over hyperrectangles in R^3 and derived sufficient conditions for the convex envelope of a sum of edge-concave functions to be equivalent to the sum of the convex envelopes of these functions. Tardella (2008) studied vertex polyhedral convex envelopes, derived sufficient conditions for their existence, and characterized their sum decomposability. This work effectively extends and unifies several results previously obtained for special cases of this problem.

2.2 Convex underestimators and relaxations

Adjiman et al. (1998a) and Hertz et al. (1999) worked on the αBB method and proposed several new rigorous methods for the calculation of the α parameters for (i) uniform diagonal shift of the hessian matrix and (ii) non-uniform diagonal shift of the hessian matrix, and they established their potential trade-offs. Adjiman et al. (1998b) presented the detailed implementation of the αBB approach and computational studies in process design problems such as heat exchanger networks, reactor-separator networks, and batch design under uncertainty. Ryoo and Sahinidis (2001) studied the bounds for multilinear functions via arithmetic intervals, recursive arithmetic intervals, logarithmic transformation, and exponential transformation, and provided comparisons of the resulting convex relaxations. Tawarmalani et al. (2002a) showed that tighter linear programming relaxations are produced if the product of a continuous variable and the sum of several continuous variables is disaggregated, and applied it to the instance of rational programs that include a nuclear reactor reload pattern design, and a catalyst mixing in a packed bed reactor problem. Tawarmalani and Sahinidis (2002b) introduced the convex extensions for lower semi-continuous functions, studied conditions under which they exist, proposed a technique for constructing convex envelopes for nonlinear functions, and studied the maximum separation distance for functions such as x/y.

Akrotirianakis and Floudas (2004a) introduced a new class of convex underestimators for twice continuously differentiable NLPs, studied their theoretical properties, and proved that the resulting convex relaxation is improved compared to the αBB one. Furthermore, Akrotirianakis and Floudas (2004b) presented computational results of the new class of convex underestimators embedded in a branch-and-bound framework for box-constrained NLPs. They also proposed a hybrid global optimization method that includes the random-linkage stochastic approach with the aim at improving the computational performance. Caratzoulas and Floudas (2005) proposed novel convex underestimators for trigonometric functions which are trigonometric functions themselves. The underestimation method can be applied to one-dimensional as well as multi-dimensional problems involving trigonometric polynomials, since the product of trigonometric functions can always be decomposed into the sum of sin and cos functions with arguments that are linear combinations of the problem variables.

Meyer and Floudas (2005b) proposed two new classes of convex underestimators for general C^2 NLPs which combine the αBB underestimators within a piecewise quadratic perturbation, derived properties for the smoothness of the convex underestimators, and showed the improvements over the classical αBB convex underestimators for box-constrained optimization problems. Sherali et al. (2005) proposed a new cutting plane methodology that is based on the construction of a partial convex hull representation for a given 0–1 mixed-integer programming problem by using the reformulation–linearization technique (RLT). The cuts are generated by projecting the extended space of the RLT formulation into the original space, and the authors investigated several variable selection rules for performing this convexification in a computationally efficient manner. Gounaris and Floudas (2008a) developed tight convex underestimators for univariate C^2-continuous functions of arbitrary structure. These are based on a piecewise application of the αBB underestimators and it is theoretically proven that a finite number of pieces is sufficient for the method to yield the—a priori unknown—convex envelope of the function. The methodology was extended to handle multivariate functions (Gounaris and Floudas 2008b), through appropriate projections of the function's epigraph into select one-dimensional spaces. Orthonormal transformations were also employed to improve the quality of the underestimation.

2.3 Convexification techniques

Tawarmalani et al. (2002b) studied $0-1$ hyperbolic programs, developed eight mixed-integer convex reformulations, proposed analytical results on the tightness of these reformulations, developed a global optimization algorithm and applied it to a p-choice facility location problem. Björk et al. (2003) studied convexifications for signomial terms, introduced properties of power convex functions, compared the effect of the convexification schemes for heat exchanger network problems, and studied quasi-convex convexifications. Li et al. (2005) discussed nonconvex minimization problems that can be equivalently transformed into convex ones, and thus be globally solved by use of only local techniques. They derived sufficient conditions for identifying such classes of problems, which are called hidden convex minimization problems. Hidden convexity was also the focus in the work by Wu et al. (2007). General convexification and concavification methods were proposed for some classes of monotone (Wu et al. 2005a) and non-monotone (Wu et al. 2005b) optimization problems, which convert them into the better structured classes of concave minimization, d.c. programming, and reverse convex programming problems.

Zlobec (2005) showed that the Liu–Floudas convexification (Liu and Floudas 1993) can be possible for every Lipschitz continuously differentiable function, practically extending the applicability of the GOP algorithm (Floudas and Visweswaran 1990) to almost every smooth program occurring in practice. Zlobec (2006) also worked on the characterization of convexifiable functions by developing necessary and sufficient conditions for the decomposition of a function into a sum of a convex and a quadratic concave function. Westerlund (2006) reviewed the work on power convex transformations that are applicable to signomial programs, the optimal exponents to be used in such an approach, the tight underestimation of the resulting program via piecewise linear approximations, and the computational framework developed for the global optimization of signomial programs. Lundell et al. (2008) presented a method for the optimal selection of the variables that need to be transformed in such a framework. The technique minimizes the number of transformations. Li et al. (2008) applied the reciprocal transformation for the convexification of posynomial programs with positive variables.

2.4 Concave, bilinear and fractional models

Zamora and Grossmann (1998b) introduced a deterministic branch-and-bound approach for structured process systems that have univariate concave, bilinear and linear fractional terms. They proposed properties for the contraction operation, embedded them in the global optimization algorithm and studied the contraction effects on several applications. Shectman and Sahinidis (1998) proposed a finite global optimization method for separable concave problems. Zamora and Grossmann (1999) proposed a branch-and-contract global optimization algorithm for univariate concave, bilinear, and linear fractional models. The emphasis was on reducing the number of nodes in the branch-and-bound tree through proper use of the contraction operator. Van Antwerp et al. (1999) studied the bilinear matrix inequality problem as a formulation of the globally optimal controller problem and applied a branch-and-bound global optimization approach to generate lower and upper bounds and prove optimality for a mass spring model and a reactive ion etching problem.

Adhya et al. (1999) studied bilinear models of the pooling problem, proposed a Lagrangian relaxation approach for the generation of valid lower bounds, and showed that these bounds are tighter when compared to linear programming based relaxations. Liang et al. (2001) presented sufficient optimality conditions and duality results, based on sublinear functionals and generalized convexity, for a class of nonlinear fractional programming problems. Ryoo and Sahinidis (2003) studied linear and generalized linear multiplicative models, applied the recursive arithmetic interval approach for the derivation of lower bounds, introduced greedy heuristics for a branch-and-reduce approach, and applied it to benchmark problems and randomly generated problems. Goyal and Ierapetritou (2003a) introduced an approach for the systematic evaluation of the infeasible domains using a simplicial outer approximation framework that is applicable to concave or quasiconvex constraints.

Benson (2004) showed how fractional programs can be reformulated so as to be solvable by parametric convex programming and concave minimization methods. Tuy et al. (2004) proposed a new approach for optimizing polynomial fractional functions under polynomial constraints. The approach is based on reformulation into a monotone optimization problem. Tsai (2005) proposed a method to solve fractional programs via convexification transformation and piecewise underestimation. Wang et al. (2005) developed a branch and bound algorithm for the global optimization of sums of several linear fractional functions over a polytope, that is based on successively refined linear relaxations. Liberti (2005) developed an automatic symbolic reformulation procedure that can uncover linearity that is embedded in bilinear programs and thus simplify such formulations. Linderoth (2005) proposed a branch-and-bound algorithm for solving nonconvex quadratically-constrained quadratic programs. The novelty of their algorithm lies in the fact that branching is done by partitioning the feasible region into the Cartesian product of two-dimensional triangles and rectangles. Explicit relaxations of the bilinear function over such triangles and rectangles are derived and used. Chinchuluun et al. (2005) developed a new approach for solving concave quadratic programming problems which is based on the improved global optimality conditions of Dur et al. (1998) and Hiriart-Urruty and Ledyav (1996).

Beck et al. (2006) derived an efficient global optimization algorithm for the regularized total least squares problem and applied it on problems arising from the inverse Laplace transform and image processing. Jiao et al. (2006) proposed solving generalized linear fractional problems via a branch and bound algorithm that is based on the construction of a linear relaxation. Benson (2006, 2007a) studied fractional programs that involve ratios of convex terms and presented a new branch and bound algorithm that requires solving a sequence of convex optimization problems. He also focused on linear sum-of-ratios problems and used a simplicial branch and bound duality-bounds algorithm to globally solve them (Benson 2007b). Nahapetyan and Pardalos (2007) presented a continuous relaxation for the Concave Piecewise Linear Network Flow Problem (CPLNFP), which has a bilinear objective function and network constraints. Ding and Al-Khayyal (2007) presented two linear cutting plane algorithms that refine methods for solving disjoint bilinear programs.

Shen and Yuan (2007) proposed a branch and bound approach for the global optimization problem of the sum of generalized polynomial fractional functions under generalized polynomial constraints. Yamamoto and Konno (2007) proposed an efficient algorithm for solving convex-convex quadratic fractional programs that combines the classical Dinkelbach approach, the integer programming approach for solving nonconvex quadratic programs, and a standard NLP solver. Nie et al. (2008) discussed the global minimization of rational functions via sum of squares relaxations. Nahapetyan and Pardalos (2008) suggested a bilinear reduction of the original MILP formulation of the capacitated multi-item dynamic pricing problem, and proposed a heuristic algorithm to solve effectively the equivalent bilinear problem.

2.5 General theoretical and algorithmic developments

Adjiman et al. (1998a,b) introduced the branch-and-bound based αBB global optimization approach, which is applicable to general twice-continuously differentiable NLPs, and presented extensive computational studies in process design problems such as heat exchanger networks, reactor-separator networks, and batch design under uncertainty. Androulakis and Floudas (1998) studied the parallel computation issues that arise using the αBB global optimization approach.

Sherali (1998) developed a relaxation–linearization technique (RLT) approach for nonconvex polynomial problems that involve mixed-sign coefficients and rational exponents, embedded it in a branch-and-bound framework, and presented suitable branching strategies that induce convergence to the global solution. Byrne and Bogle (1999) introduced a bound constrained linear relaxation, developed two classes of linear underestimators using the natural extension and mean value theorems of interval analysis, and showed that the interval LP is more efficient than other interval analysis approaches. Xu et al. (2001) studied filled function techniques for unconstrained global optimization and presented more general forms of filled functions for smooth and non-smooth optimization. They derived conditions on the forms of functions and on the values of their parameters, so that they have the desired properties of filled functions. Sherali and Wang (2001) combined the RLT with approximation-generated linear relaxations, developed a branch and bound framework for the global optimization of general nonconvex factorable problems, and applied their method on fifteen engineering process control and design test problems from various literature sources. Sherali and Fraticelli (2002) proposed a mechanism for the tightening of RLT relaxations through semidefinite cutting planes. The approach is based on replacing the nonnegativity restrictions on the matrix of RLT product variables by a positive semidefinite constraint, which is relaxed suitably to provide this new class of cuts. The authors reported significant improvement in the tightness of the relaxation when compared with a standard RLT approach.

Gau and Stadtherr (2002a) studied the computational improvement of interval Newton with generalized bisection approaches, introduced a hybrid preconditioning strategy where a pivoting preconditioner is combined with the standard inverse midpoint method, and showed that this approach results in a large reduction of the needed subintervals and hence in significant computational improvements. Gau and Stadtherr (2002b) studied synchronous work stealing, synchronous and asynchronous diffusive load balancing on a two-dimensional torus virtual network, developed a distributed computing interval Newton framework, and showed that superlinear speedups can be obtained for vapor–liquid equilibrium and parameter estimation problems.

Lucia and Feng (2002) studied the least squares function landscape, introduced a differential geometry based framework for the determination of all physically meaningful solutions, singular points, and their connectivity, developed a global terrain algorithm, and illustrated the framework through one and two-dimensional examples from glass temperature calculations, equilibrium states in nanostructured materials, a simplified SAFT equation, and a CSTR equation. Lucia and Feng (2003) extended the terrain methodology to multivariable problems and integral curve bifurcations associated with valleys and ridges, showed that the terrain methods are superior to arc homotopy continuation in the presence of parametric disconnectedness, and studied examples for the location of all azeotropes, retrograde flash calculations, and CSTR problems.

Casado et al. (2002) developed three new algorithms based on interval analysis and branch-and-bound global optimization approaches to solve the problem of finding the smallest root of an one-dimensional function. The novelty of these methods is in improving the elimination criteria and the order in which interval and point evaluations are performed, thus realizing greater computational efficiency than existing interval root-finding methods. Their approach was also extended so as to handle multiextremal and nondifferentiable functions. Casado et al. (2003) proposed new interval analysis support functions. These enable one to develop more powerful bounding, selection, and rejection criteria, which result in significant coputational savings. They applied their enhancements on a wide set of multiextremal test functions, and reported that the new algorithm works almost two times faster than a traditional interval analysis global optimization method. A natural n-dimensional extension to these algorithms was later presented by Martinez et al. (2004). Zilinskas and Bogle (2003) studied the evaluation of ranges of functions through balanced random interval arithmetic, investigated the hypothesis on the normal distribution of the centers and radii of the evaluated balanced random intervals through several computational studies, and concluded that this hypothesis is incorrect.

Zhu and Fu (2003) developed a sequential convexification method (SCM) for continuous global optimization problems that is based on a simple transformation to convert the objective function into an auxiliary function with gradually fewer number of local minimizers. The method requires use of only local techniques and with probability one converges asymptotically to a global minimizer. Gao (2003, 2004) presented detailed applications of the canonical dual transformation method in quadratic and d.c. programming. Based on the same method, Gao (2005) also presented a duality theory for solving concave minimization problems subject to nonlinear inequality constraints, and polynomial programming problems subject to box constraints (Gao 2007). Sun et al. (2005) considered four classes of augmented Lagrangian functions and presented new results on the existence of their saddle points. The findings provide new insights to the role played by augmented Lagrangians in local duality theory of constrained nonconvex optimization. Borradaile and Van Hentenryck (2005) worked on how to derive safe linear relaxations to account for numerical errors due to the underlying floating-point environment of the calculations. They derived two classes of safe linear estimators for univariate functions, studied their tightness, and combined them to derive estimators for the multivariate case.

Floudas and Jongen (2005) considered the minimization of smooth functions in the Euclidean space with a finite number of stationary points having moderate asymptotic behavior at infinity, and emphasized the crucial role of saddle points. They showed that, in general, any two local minima can be connected via an alternating sequence of local minima and transition points of first order. Shen (2005) developed a linearization method for the global optimization of generalized geometric programs (GGPs). Through a sequence of linear programming problems, the method is proven to be convergent to the global optimum of the original nonconvex problem. Wang and Liang (2005) applied a combination of a branch-and-bound method with a cutting-plane method to globally solve GGPs after their tranformation to reverse convex programming problems. Li and Tsai (2005), Tsai and Lin (2006), and Tsai et al. (2007) studied generalized GGPs in the presence of non-positive variables, proposed a technique for treating these variables, and provided convexification rules for certain signomial terms. Tsai and Lin (2007) applied this work and developed an algorithm to find all solutions of systems of nonlinear equations with free variables.

Marcovecchio et al. (2006) presented a new algorithm for nonconvex NLPs that is based on the solution of two problems, called the reformulated and the main problem. The former is a suitable reformulation of the original and involves only convex and univariate concave terms, while the latter is a valid convex relaxation. Parpas et al. (2006) proposed a stochastic algorithm for the global optimization of nonconvex functions over a polytope. Their method follows the trajectory of an appropriately defined stochastic differential equation. They also studied the global optimization of robust chance constrained problems (Parpas et al. 2008), assuming that the probability measure with which the constraints are evaluated is known only through its moments. Hirsch et al. (2007) extended the GRASP algorithm (Feo and Resende 1989, 1995) of discrete optimization to continuous problems, and applied this stochastic heuristic to two hard global optimization problems. Li et al. (2007) proposed a class of general transformation methods to convert a nonconvex problem to an equivalent one for which, under certain assumptions, the existence of a local saddle point of its Lagrangian function can be guaranteed.

Floudas and Kreinovich (2007a,b) showed that natural symmetry requirements enable one to analytically solve the problem of finding the optimal functional forms for convex underestimators for twice continuously differentiable functions, and identified the original (Adjiman et al. 1998a,b) and the generalized (Akrotirianakis and Floudas 2004a,b) αBB method as the only optimal schemes that satisfy such a requirement. Gounaris and Floudas (2008c) developed sufficient convexity conditions for products of univariate functions. The results also provide insight on why transformations already proposed in the literature, like the exponential (Maranas and Floudas 1997) or the reciprocal (Li et al. 2008), actually work in the convexification of posynomial programs. A novel global optimization method based on an augmented Lagrangian framework was introduced by Birgin et al. (2008). They utilize the αBB method to ϵ-globally solve the subproblems that are generated at each outer iteration.

2.6 Application-oriented developments

Yamada and Hara (1998) proposed a global optimization approach based on the triangle covering for H-infinity control with constant diagonal scaling. Sherali et al. (2001) studied the water distribution network design problem. They developed two global optimization approaches, one based on polyhedral outer approximation and the other on the reformulation–linearization technique (RLT), and solved three standard test problems and a real problem to proven global optimality.

Westerberg and Floudas (1999a,b) introduced a global optimization framework for the enclosure of all transition states of potential energy hypersurfaces, and studied the reaction pathways and dynamics of helical formation with and without solvation. Wales and Scheraga (1999) described the progress in finding the global minima of potential energy functions. Their focus was on applications of the basin-hopping approach to atomic and molecular clusters, as well as more complicated hypersurface deformation techniques for crystals and biomolecules—methods that have produced promising results. Sherali et al. (2002) studied the capacitated Euclidean distance location–allocation problems, reported that an RLT approach leads to superior lower bounds than those computed via a projected location space subproblem, tightened further their relaxation by incorporating certain-cut-set inequalities and objective function based cuts, and extended their approach to the general $l(p)$ distance problem.

Klepeis et al. (1998) and Klepeis and Floudas (1999a) proposed new global optimization approaches for the structure prediction of solvated peptides using area and volume accessible to the solvent models. Klepeis and Floudas (1999b) proposed also a novel deterministic global optimization approach for free energy calculations of peptides. Klepeis et al. (1999) introduced a novel approach that combines deterministic global optimization and torsional angle dynamics for the prediction of peptide structures using a sparse set of NMR data. Klepeis et al. (2002) presented the advances in deterministic global optimization based on the αBB approach and its applications for structure prediction of oligopeptides, dynamics of helical formation, and protein–peptide interactions. Klepeis and Floudas (2003a) introduced a deterministic global optimization approach, αBB coupled with torsional angle dynamics, for the protein structure prediction given restraints predicted from the identification of α-helices and β-sheets. Klepeis and Floudas (2003b) proposed Astro-Fold, a first principles framework for the protein structure prediction. They described the global optimization and mixed-integer optimization advances, and presented a variety of test systems including several blind protein predictions. Klepeis et al. (2003a) introduced a new class of hybrid global optimization methods denoted as integrated hybrids for the oligopeptide structure prediction. Klepeis et al. (2003b) proposed new alternating hybrid global optimization methods, studied and developed their distributed computing algorithms, and applied them to the structure prediction of met-enkaphalin and mellitin. These two classes of hybrid global optimization approaches combine the αBB for the generation of rigorous lower bounds with the modified genetic algorithm, CSA, for the upper bounding calculations. Reviews of the global optimization activities in the areas of protein folding and peptide docking can be found in Floudas (2005, 2007) and Floudas et al. (2006).

Doye et al. (2004) developed new transformation techniques to improve the global optimization of models that include Morse potentials and, thus, aid the study of biomolecules. Schafroth and Floudas (2004) studied the protein–peptide interactions via deterministic global optimization, atomistic-level modeling, and several solvation methods that include the area accessible to the solvent, the volume accessible to the solvent, and the Poisson–Boltzmann method, and reported excellent agreement on the binding motifs. Moloi and Ali

(2005) proposed an algorithm for minimizing potential energy functions that is based on the differential evolution algorithm by Storn and Price (1997), and tested it on two different types of potentials.

Bringas et al. (2007) worked on the optimal design of groundwater remediation networks that use selective membranes for the valorization of anionic pollutants. They globally solved select instances of their superstructure using a Lagrangean decomposition algorithm. Maringer and Parpas (2008) proposed an extension of the Markowitz mean variance model for the global optimization of the higher moments in portfolio selection, which they solved using two stochastic algorithms based on differential evolution. Gattupalli and Lucia (2008) applied a multi-scale global optimization methodology, based on terrain methods and funneling algorithms, to find the minimum energy molecular conformations of pure n-alkanes. The results are indicative of typical fuel oils and useful in understanding the waxing of petroleum fuels. Amaral et al. (2008) developed an RLT-based algorithm for the global optimization of a nonconvex problem that arises in total least squares with inequality constraints, and in the correction of infeasible linear systems of equalities. Kallrath (2008) studied the simultaneous packing of circles and polygons in rectangles, using global optimization approaches.

2.7 Phase equilibrium

Maier et al. (1998) applied an interval analysis based approach for the enclosure of homogeneous azeotropes. They employed the formulations proposed by Harding et al. (1997) and studied systems with activity coefficient and equation of state models. Meyer and Swartz (1998) proposed a new approach for testing convexity for phase equilibrium problems. McKinnon and Mongeau (1998) proposed a generic global optimization approach for the phase and chemical reaction equilibrium problem that is based on interval analysis and combines the stability criterion with the minimization of the Gibbs free energy. Hua et al. (1998a) applied an interval analysis method for the phase stability computations of binary and ternary mixtures using equation of state models. They introduced also two enhancements on their approach based on monotonicity and mole fraction weighted averages for improving the efficiency in the tangent plane stability analysis for cubic equations of state (Hua et al. 1998b).

Zhu and Xu (1999a) used simulated annealing for the tangent plane stability analysis criterion and they applied it to ternary systems. They studied also the tangent plane stability analysis for the SRK cubic equation of state through a Lipschitz global optimization approach, and applied it to binary systems (Zhu and Xu 1999b). Moreover, they used simulated annealing for the stability analysis of liquid-liquid equilibrium systems modeled via the NRTL and UNIQUAC equations for the activity coefficients and studied ternary systems with up to three liquid phases (Zhu and Xu 1999c).

Harding and Floudas (2000a) introduced a novel global optimization approach for the phase stability of several cubic equations of state based on analytical findings and the principles of the αBB global optimization framework. Harding and Floudas (2000b) studied the enclosure of all heterogeneous and reactive azeotropes, developed a rigorous framework based on the αBB global optimization principles, and demonstrated its potential for a variety of case studies. Tessier et al. (2000) introduced monotonicity based and mole fraction weighted averages based enhancments for the application of interval Newton methods to the phase stability problem using the NRTL and UNIQUAC models. Zhu et al. (2000) proposed an enhanced simulated annealing algorithm for the tangent plane stability problem using the PR and SRK cubic equations of state.

Zhu and Inoue (2001) introduced a branch-and-bound approach based on a quadratic underestimating function and applied it to the tangent plane distance criterion using the NRTL equation. Xu et al. (2002) studied the phase stability criterion using the SAFT equation of state, introduced an interval Newton/generalized bisection approach, followed a volume-based formulation based on the Helmholtz energy, and applied to nonassociating, self-associating, and cross-associating systems. Cheung et al. (2002) studied the global minimum determination of clusters for the solvent-solute interactions in phase equilibrium. They introduced the OPLS force field, derived tight convex underestimators, derived bounds on the dependent variables, developed a branch-and-bound approach, and applied it to a butane molecule and a butane-ethylamine system.

Scurto et al. (2003) developed a methodology to predict the behavior of high-pressure solid-fluid equilibrium systems with cosolvents, where the likelihood of formation of more than two phases is great. Lin and Stadtherr (2004a) applied their interval-Newton procedure, enhanced by a new LP bounding strategy, on various phase equilibrium problems. Nichita et al. (2004) used the tunneling global optimization method to directly minimize the Gibbs free energy in multiphase equilibria calculations. Nichita et al. (2006) used the same method to solve the nonconvex phase stability problem that results from the tangent plane distance criterion in terms of the Helmholtz free energy. Henderson et al. (2004) formulated an optimization problem based on a slight modification of the Gibbs tangent plane criterion, and used a simulated annealing algorithm to solve it. Freitas et al. (2004) studied a number of binary mixtures by solving the aforementioned formulation. They used a novel and robust algorithm that does not require use of derivatives and is insensitive to the quality of initial guesses. Lucia et al. (2005) incorporated new ideas within the terrain methods to study the phase stability and equilibrium of n-alkanes. Srinivas and Rangaiah (2006) evaluated their implementation of the random tunneling algorithm on a number of medium sized problems, including VL, LL, and VLL phase equilibrium problems. Srinivas and Rangaiah (2007) also focused on solving phase equilibrium problems with differential evolution and tabu search methods. They reported better performance when the methods are combined and a tabu list is used in the generation step of differential evolution. Mitsos and Barton (2007) reinterpreted the Gibbs tangent plane stability criterion via a Lagrangian duality approach, and performed case studies based on the NRTL and UNIQUAC activity coefficient model.

2.8 Parameter estimation

Esposito and Floudas (1998) studied the error-in-variables approach and proposed the first global optimization method for the parameter estimation and data reconcilliation of nonlinear algebraic models using the principles of the αBB approach. Gau and Stadtherr (2000) introduced an interval analysis based approach for the error-in-variables method and studied vapor liquid equilibrium and reaction kinetics models. Gau et al. (2000) studied further the parameter estimation of vapor liquid equilibrium models via interval analysis, applied it using the Wilson equation for a variety of binary systems, and demonstrated that correct predictions of azeotropes are attained only based on the global optimum parameter solutions in direct contrast to the Dechema data collection.

Gau and Stadtherr (2002c) applied the interval-Newton approach for the parameter estimation of a catalytic reactor model, a heat exchanger network model, and binary vapor–liquid equilibrium problems using the Wilson equation, and pointed out that problems of about two hundred variables can be addressed. Lin and Stadtherr (2004b) proposed a linear programming bounding scheme that enhances the performance of the interval-Newton method, and applied the new technique on parameter estimation problems. Ulas et al. (2005) studied the uncertainties in thermodynamic models that result from parameter estimation. Their results identified errors in published thermodynamic data collections and can improve the performance of batch distillation controllers. Singer et al. (2006) presented a method that can find the best possible least-squares fit of experimental data by a nonlinear kinetic model.

3 Mixed-integer nonlinear optimization

This section lists recent publications in areas of mathematical programming that involve discrete components. The entries are classified into theoretical and implementation contributions for MINLP, formulation of MINLP models and studies of particular problems, and advances in the area of generalized disjunctive programming (GDP). As this classification is not mutually exclusive, some publications could have appeared in more than one subsections.

3.1 MINLP: theoretical and algorithmic developments

Zamora and Grossmann (1998a) derived thermodynamic-based convex underestimators, quadratic and linear fractional convex underestimators, and proposed a hybrid branch-and-bound and outer approximation method for the global optimization of heat exchanger networks with no stream splits. Sherali et al. (1998) presented an extension of the reformulation–linearization technique (RLT) that is designed to exploit special structures. This framework permits the generation of successively tighter relaxations, leading up to the convex hull representation. The authors explored also the strengthening of the RLT constraints through conditional logical expressions, as well as relationships with sequential lifting.

Westerlund et al. (1998) proposed an extended cutting plane approach for the global optimization of pseudoconvex MINLP problems, studied its convergence properties, and applied it to an example from the paper-converting industry. Pörn et al. (1999) proposed convexification schemes for classes of discrete and integer nonconvex models. They studied the exponential transformation and potential-based transformations and applied them to integer posynomial problems. Pörn and Westerlund (2000) introduced procedures for the successive linear approximation of the objective function and line search techniques, proposed a cutting plane method for addressing global MINLP problems that feature pseudo-convex objective function and constraints, studied its convergence properties and initialization schemes, and tested it on several benchmark problems arising in process synthesis and scheduling applications.

Adjiman et al. (2000) proposed two novel global optimization approaches for nonconvex mixed-integer nonlinear programming problems. The first approach, SMIN–αBB is for separable continuous and integer domains and it is based on the principles of αBB type of convex underestimators and a branch-and-bound approach for the mixed set of continuous and binary variables. The second approach, GMIN–αBB, is applicable to general mixed integer nonlinear problems which are not separable in the continuous and integer variables, and it is based on a branch-and-bound tree constructed only in the integer domain while the αBB principles are used to solve the nonconvex NLPs at each node so as to generate valid lower bounds. The first approach was applied to heat exchanger network problems, while the second one was applied to pump network configuration problems and trim loss minimization problems in addition to a variety of benchmark problems. Kesavan and Barton (2000) introduced a generalized branch-and-cut algorithm for nonconvex MINLPs, showed that decomposition-based approaches and branch-and-bound algorithms are special cases, and proposed a number of heuristics towards addressing the computational efficiency issues. Sherali et al. (2000) explored the generation of reduced first-level RLT representations, showed that there exist representations with about half the constraints of the full first-level representation whose relaxations yield the same lower bound value, and argued that an accurate a priori prediction of the form of such representations is not always achievable.

Ostrovsky et al. (2002) studied nonconvex MINLP models in which most variables are in the nonconvex terms and the number of linear constraints is much larger than the nonlinear constraints, introduced the idea of branching on a set of linear branching variables which depend linearly on the search variables, proposed a tailored branch and bound approach using linear understimators for tree functions based on a multilevel function representation, showed that there is a significant reduction in the branching variable space, and applied it to solvent design and recovery problems. Dua et al. (2002) proposed novel approaches for multiparametric mixed-integer quadratic models through the decomposition into a multiparametric quadratic MIQP model for the upper bound and a potentially nonconvex MINLP model for the lower bound, suggested ways of addressing the nonconvexity in the MINLP, and generated envelopes of parametric solutions and the enclosure of the multiparametric MIQP. They applied their method in model predictive and hybrid control problems. Zhu and Kuno (2003) proposed a hybrid global optimization method for nonconvex MINLPs which combines convex quadratic underestimation techniques with a revised form of the generalized Benders decomposition, suggested its convergence properties, and illustrated it via a two variable problem. Goyal and Ierapetritou (2003b) studied MINLP models where the objective function is convex, and the constraints are convex, concave or quasi-concave, introduced the simplicial approximation of the convex hull of the feasible region, proposed algorithmic procedures and illustrated them via small benchmark problems.

Yan et al. (2004) extended the line-up competition algorithm to handle integer variables, and tested its performance with several nonconvex MINLP problems published in the literature. Dua et al. (2004) studied issues concerning the solution of parametric nonconvex programs, proposed a branch and bound algorithm, and discussed the need for defining a suitable overestimating subproblem. Tawarmalani and Sahinidis (2004) developed a branch and bound framework for the global optimization of continuous, integer, and mixed-integer nonlinear programs. It involves novel linear relaxation schemes, a Lagrangian/linear duality-based theory for domain and range reduction, as well as branching strategies that guarrantee finiteness of the solution sequence for certain classes of problems. They also discuss implementation issues and present computational results with a variety of benchmark problems. Kesavan et al. (2004) studied separable MINLP models with nonconvex functions, proposed two decomposition algorithms based on alternating sequences of relaxed master problems, two nonlinear programming problems, and outer approximation, showed that the first algorithm yields the global solution while the second provides a rigorous bound on the global solution, and presented computational results on several benchmark problems and heat exchanger network problems.

Chaovalitwongse et al. (2004) considered the reduction of multi-quadratic 0–1 programming problems to linear mixed 0–1 programming problems, with a reformulation that limits the number of required continuous variables. Prokopyev et al. (2005a,b) considered single- and multiple-ratio unconstrained hyperbolic 0–1 programming problems, proved that checking for the uniqueness of their solution is NP-hard, and discussed the complexity of local search and the approximability of multiple-ratio problems. Prokopyev et al. (2005b) studied also their MILP reformulations, and presented a GRASP-based heuristic for solving cardinality constrained problems. Tawarmalani and Sahinidis (2005) introduced a polyhedral branch-and-cut approach in global optimization. Their algorithm exploits convexity in order to generate the polyhedral cuts and relaxations for multivariate nonconvex problems.

Computational results with a collection of benchmark NLP and MINLP problems were presented. Munawar and Gudi (2005) proposed a hybrid method that combines stochastic and deterministic approaches to improve the convergence rate of differential evolution (DE) algorithms, and utilized a nonlinear transformation proposed in the literature so as to more effectively take into account the integrality restrictions of the integer variables in an MINLP formulation. In the context of linear and polynomial MIP problems, Adams and Sherali (2005) used Lagrange interpolating polynomials to generalize the level-1 RLT constraints for a binary variable to the general discrete case.

Zhu and Kuno (2006) developed a cutting-plane branch-and-cut algorithm for the solution of convex MINLPs. The method utilizes the lift-and-project technology, which accelerates the branching process by generating cuts through the solution of a transformed projection problem. The computational results indicate that the method can address large-scale problems. Luo et al. (2007) developed an improved particle swarm optimization (PSO) algorithm for solving nonconvex MINLPs. The algorithm includes a transformation procedure where mixed variables are partitioned and reduced variables are identified through analyzing and tearing equality constraints. In addition, the discrete variables are updated independently according to a given criterion and not simultaneously with the continuous ones. Young et al. (2007) proposed the implementation of information theory to the mutation stage of a genetic algorithm so as to refresh the premature population. The novel algorithm, called information-guided genetic algorithm (IGA), can address general MINLPs and does not require any additional number of variables and constraints or knowledge of an initial feasible point. Computational results on a variety of problems show superior convergence and global minimum discovery rates than traditional genetic algorithm methods. Pardalos et al. (2008) used global equilibrium search techniques for the solution of benchmark unconstrained binary quadratic optimization problems, studied their computational efficiency, and reported better performance when compared with multistart tabu search methods. Based on the canonical dual transformation (Gao 2004), Fang et al. (2008) constructed a pair of canonical dual problems for the 0–1 quadratic programming problem, showed that no duality gap exists, derived optimality conditions of both the local and global type, and developed an algorithm for large scale problems.

3.2 MINLP: formulations and applications

Sinha et al. (1999) studied the class of solvent design problems, modelled it as a nonconvex MINLP problem, identified the sources of nonconvexities in the properties and solubility parameter design constraints, proposed linear underestimators based on a multilevel representation approach for the functions, developed a reduced space branch-and-bound global optimization algorithm, and applied it to a single component blanket wash design problem. Noureldin and El-Halwagi (1999) studied mass integration problems for pollution prevention, proposed targets for the maximum achievable pollution, introduced an interval analysis framework for the determination of these targets, studied the pollution prevention via unit manipulation, recycle and interception, and employed the interval-based targets in a case study featuring the reduction of water usage and discharge in a tire-to-fuel plant. Harjunkoski et al. (1999) studied the trim loss minimization problem for the paper converting industry, formulated it as a nonconvex MINLP, proposed transformations for the bilinear terms that are based on linear representations and convex expressions, studied the reductions of the combinatorial space, investigated the role of different types of objective functions, developed and assessed several algorithmic alternatives, and showed that the global solution can be obtained with all strategies and certain convex formulations performed similarly to the linear models.

Sahinidis and Tawarmalani (2000) presented two MINLP applications of global optimization for the design of just-in-time flowshops, and the design of an alterative to freon. In the first study, the model determines the stagewise number of machines needed that minimizes the total equipment costs, and they showed improvements compared to the heuristic approaches. In the second study, the model selects the constituent parts of a molecule so as to satisfy chemical and physical properties, economic, environmental constraints through a group contribution based approach, and provides a ranked order list of alternative compounds. Parthasarathy and El-Halwagi (2000) studied a systematic framework for the optimal design of condensation which an important technology for volatile organic compounds, formulated it as a nonconvex MINLP model, proposed an iterative global optimization approach which is based on physical insights and active constraint principles that allow for decomposition and efficient solution, and applied it to a case study for the manufacture of adhesive tapes.

Björk and Westerlund (2002) studied the global optimization of heat exchanger network synthesis through the simplified superstructure representation that allows only series and parallel schemes, applied convexification approaches for signomials via piecewise linear approximations, developed convex MINLP lower bounding models using the Patterson formula for the log mean temperature difference considering both isothermal and nonisothermal mixing, proposed a global optimization approach for alternative models, and presented extensive computational studies. Wang and Achenie (2002a) studied solvent design problems which are formulated as nonconvex MINLPs, introduced a hybrid global optimization approach which combines outer approximation with simulated annealing, applied it to several benchmark problems, case studies for the extraction of acetic acid from water, and solvent design for reversible reactions, and showed that near optimal solutions can be located. Wang and Achenie (2002b) studied also the molecular design of solvents for extractive fermentation including solvent attributes such as biocompatibility, inertness and phase splitting, introduced a group contribution framework which results in a nonconvex MINLP model, studied a local MINLP algorithm, OA/ER/AP, and applied it to case studies on ethanol extractive fermentation.

Ostrovsky et al. (2003) revisited their molecular design reduced dimension branch-and-bound algorithm by studying further the branching functions concept and the special tree function representation, proposed the sweep method for the construction of the linear underestimators, investigated the problem size dependency on the algorithmic performance, and showed that the computational effort increases almost linearly. Vaia and Sahinidis (2003) studied the simultaneous parameter estimation and model structure identification in infrared spectroscopy, proposed two methods out of which the second corresponds to a single nonconvex MINLP model, presented a branch-and-bound approach which is based on a relaxation of terms that are logarithmic, bilinear, and multilinear depending on the determinant of the covariance matrix, and presented comparative computational results. Sinha et al. (2003) studied the systematic design of cleaning solvent blends for lithographic printing, modelled it as a nonconvex MINLP problem, introduced an interval analysis based global optimization approach with modifications on the upper bounding calculation and the local feasibility test which are solved via SQP, and an interval-based domain reduction algorithm, and presented computational results for the design of aqueous blanket wash blends. Sahinidis et al. (2003) revisited the design of alternative refrigerants problem, introduced an integer formulation for previously described structural constraints, proposed new structural constraints between one-bonded and higher-bonded groups in the absence of rings and new clique constraints for rings, applied a branch-and-reduce global optimization algorithm with a modification so as to generate all feasible integer solutions, and generated new compounds for refrigerants. Kallrath (2003) studied and solved a nonconvex product portfolio problem via an approximate MILP formulation of the objective function and exact linear relations for the constraints, modelled it as a nonconvex MINLP problem for the optimization of the number and size of batch process units, analyzed the sources of nonconvexity consisting of concave functions and trilinear products, investigated the piecewise linear approximation of the objective function, the use of a local MINLP solver, SBB, and a global optimization solver, Baron, and reported that for the large instances weak lower bounds are generated.

Pardalos et al. (2004) formulated a quadratically constrained 0–1 programming problem to identify critical brain electrode sites that are relevant in the detection of precursors to temporal lobe seizures. They reported the first analysis of an automated online algorithm for detecting these precursors in ongoing EEG signals, effectively providing a prospective seizure warning system. Emet and Westerlund (2004) conducted a computational comparison of solving a cyclic chromatographic separation problem using MINLP methods, and reported that the extended cutting plane (ECP) method compares favourably against traditional outer approximation and branch-and-bound methods. A review of the recent advances on MINLP optimization of planning and design problems in the process industry was presented by Kallrath (2005).

Ghosh et al. (2005) studied mixed-integer formulations for the identifications of metabolic network fluxes via NMR data. They proposed a joint problem methodology that involves using the MILP solutions of the "front end" analysis to bound the desired solution of the data-to-fluxes problem. A branch-and-bound global optimization algorithm was used to solve the latter. Lin et al. (2005) revisited the nonconvex product portfolio problem introduced by Kallrath (2003), presented an improved formulation consisting of a concave objective function with linear constraints in the continuous and binary variables, proposed several techniques for tightening the model and accelerating its solution, developed a customized branch-and-bound approach which addresses the problem to global optimality, applied it to small and large instances, and demonstrated that global solutions can be obtained very efficiently in contrast to commercial MINLP solvers. Based on global equilibrium search techniques, Pardalos and Shylo (2006) proposed an algorithm to solve the job shop scheduling problem, and reported improved upper bounds for several well-known benchmark problems.

Sherali and Desai (2005a) formulated the hard clustering problem as a mixed-integer nonlinear program and solved it to global optimality with use of the RLT. The authors applied their method to a number of standard data sets found in the literature, as well as on larger problem instances which they synthesized, and reported robustness of the procedure and computational dominance over the k-means algorithm. They also developed a root-node heuristic procedure to reach a good quality solution early in the branch and bound process. The methodology was extended later to address also the fuzzy clustering problem (Sherali and Desai 2005b).

Meyer and Floudas (2006) studied superstructures of pooling networks, which are important to the petrochemical, chemical, and wastewater treatment industries, and formulated this generalized pooling problem as a nonconvex MINLP that involves many bilinear terms in the constraint functions. They proposed a global optimization algorithm that is based on a novel piecewise linear reformulation–linearization technique (RLT) formulation that they developed. Using this approach, the authors were able to verify the global solution of a combinatorially complex industrial problem that contained 156 bilinear terms and 55 binary variables. Karuppiah and Grossmann (2006) addressed the problem of optimal synthesis of an integrated water system, where water using processes and water treatment operations are jointly taken into account. The resulting MINLP was solved with a new deterministic spatial branch and contract algorithm, in which piecewise under- and over-estimators are used for constructing the relaxations at each node. The extension of the model to include the uncertainty in various operating parameters was presented in a later publication

(Karuppiah and Grossmann 2008a). The extended MINLP is a deterministic equivalent of a two-stage stochastic programming model with recourse, where the uncertain parameters take on a finite number of realizations. This problem is addressed with a spatial branch-and-cut algorithm that uses Lagrangian decomposition (Karuppiah and Grossmann 2008b). Karuppiah et al. (2008) presented an outer-approximation algorithm to globally solve a nonconvex MINLP formulation that corresponds to the continuous-time scheduling of refinery crude oil operations. The solution procedure relies on effective MILP relaxations that benefit from additional cuts derived after spatially decomposing the network.

Bergamini et al. (2007) formulated an MINLP model for the global optimization of heat exchanger networks, and presented a new solution methodology that is based on outer approximation and utilizes piecewise underestimation. Rigorous constraints obtained from physical insights are also included in the formulation, and the authors reported computationally efficient global solutions for problems with up to nine process streams. Foteinou et al. (2008) presented a mixed-integer optimization framework for the synthesis and analysis of regulatory networks. Their approach integrates prior biological knowledge regarding interactions between genes and corresponding transcription factors, in an effort to minimize the complexity of the problem. The original nonconvex formulation is appropriately linearized and the resulting MILP solved with use of standard commercial solvers. A case study involving gene expression and binding data from *E.coli* is presented.

Tan et al. (2007a) presented a novel clustering approach for use with DNA microarray data. The algorithm is based on the Global Optimum Search methodology (Floudas et al. 1989; Floudas 1995) and includes a procedure to determine the optimal number of clusters to be used. The approach compared favourably with other methods, in terms of intra-cluster similarity and inter-cluster dissimilarity, when it was applied on a case study that involves data centered on the Ras signaling pathway of *S. cerevisiae*. Tan et al. (2007b) also studied the effects of different normalization and pre-clustering techniques on the clustering results produced with the previous approach. They reported that these can be significant and should be taken into consideration when attempting to cluster microarray data and, therefore, this work has significance in fine-tuning their novel clustering approach discussed above.

Rebennack et al. (2008) proposed a decomposition algorithm for the special class of MINLPs that have an assignment constraint, and formulated the column enumeration approach. The resulting master problem is a partitioning problem whose objective function coefficients are computed via easy-to-solve optimization subproblems. They applied the method on a problem of packing circles into several given rectangles. Exler et al. (2008) studied MINLP formulations with differential-algebraic constraints that arise in the integrated design of process and control systems. In order to globally solve this class of problems, they developed extensions of the metaheuristic Tabu Search. They applied their method on a wastewater treatment plant model (Alex et al. 1999) and the Tennessee Eastman Process (Downs and Vogel 1993).

3.3 Generalized disjunctive programming, GDP

Vecchietti and Grossmann (1999) introduced a disjunctive programming approach for MINLPs, denoted as LOGMIP, discussed a hybrid modeling framework for process systems engineering which allows both binary variables and disjunctions as tools for discrete decisions, implemented a modified logic-based outer approximation approach, and presented computational studies on two process synthesis problems and an FTIR spectroscopy example. Lee and Grossmann (2001) studied nonconvex generalized disjunctive programming models, constructed the convex hull of each nonlinear disjunction, used convex underestimators for bilinear, linear fractional and concave separable functions, introduced a two level branch-and-bound algorithm where the lower bound requires a discrete search in the disjunctions space and the upper bound requires a spatial divide and conquer search in the nonconvex continuous space, and applied it to benchmark problems, a multicomponent separation problem, multistage design/synthesis of batch plants with parallel units, and heat exchanger network synthesis.

Grossmann and Lee (2003) studied generalized disjunctive programming, GDP, problems which feature convex nonlinear inequalities in the disjunctions, proposed a convex nonlinear relaxation of the nonlinear GDP problem based on the convex hull representation of each of the disjunctions which was derived by variable disaggregation and reformulation, formulated the nonlinear GDP as an MINLP which was shown to produce improved bounds compared to big-M models, and presented comparative computational studies of the two formulations. Lee and Grossmann (2003) studied nonconvex GDP problems with bilinear equality constraints, derived convex underestimators and overestimators for the bilinear constraints using the reformulation/linearization approach, expressed the discrete choices as disjunctions which were subsequently relaxed by their convex hull representations, used their earlier two level global optimization approach (Lee and Grossmann 2001), and presented computational studies for pooling problems, water usage problems, and wastewater network problems. Vecchietti et al. (2003) presented characterization and properties for various types of disjunctions, including an interesting result for improper disjunctions. They proposed also a cutting plane method that avoids the explicit generation of equations and variables of the convex hull, and used this method to solve a small process synthesis problem.

Montagna et al. (2004) formulated a generalized disjunctive programming model to address the problem of synthesis of a biotechnological process in which a set of biotechnological products must be elaborated. They solved the problem after transforming it into an MINLP with use of either a big-M or a convex hull reformulation, and they evaluated the computational performance of the two approaches. Stein et al. (2004) proposed different alternatives to address the combinatorial component of GDP and MINLP models and reformulate them into continuous optimization problems, investigated theoretical properties of the various reformulations with regard to their numerical solution, and demonstrated their results with process engineering applications that involve stationary as well as dynamic process models.

Lee and Grossmann (2005) presented a review of advances in the area of discrete/continuous mathematical programming. After a brief presentation of algebraic-based MILP and MINLP approaches, the authors focused on the alternative approach of logic-based GDP modeling. They reviewed various solution strategies, a hybrid model that integrates disjunctive with mixed-integer programming, as well as their two-level branch-and-bound procedure for the global optimization of nonconvex GDP problems. Sawaya and Grossmann (2005) discussed issues regarding the computational implementation of the convex hull reformulation for nonlinear generalized disjunctive programming. In particular, they addressed the issue of division-by-zero avoidance in the inequalities representing the convex hulls, while preserving the convexity of the problem. They proposed to replace the original set of constraints with two approximating constraint sets, and they strengthened their approach by deriving theoretical conditions under which one of the sets is superior to the other. Sawaya and Grossmann (2007) also proposed a cutting plane method for solving linear generalized disjunctive programming problems. The method relies on cuts generated by an LP or QP separation problem that successively strengthen the equivalent big-M reformulation of the original GDP problem. The authors provided illustrative examples in the areas of strip-packing, retrofit planning, and zero-wait job-shop scheduling.

4 Differential-algebraic models, DAEs

Esposito and Floudas (2000a) studied the global optimization in parameter estimation of systems described by differential-algebraic models, proposed a rigorous global optimization approach based on a collocation framework and the αBB principles, proposed a global optimization approach based on an integration framework, and investigated a variety of benchmark problems and complex kinetic mechanisms. Esposito and Floudas (2000b) studied the deterministic global optimization of nonlinear optimal control problems, introduced the integration-based framework, investigated the properties of the input–output map of solutions, suggested three alternative ways of calculating the β values for the lower bounding problems, and demonstrated through several challenging case studies the algorithmic trade-offs of the different strategies, as well as the determination of the global solution. Barton et al. (2000) studied the optimization of hybrid discrete/continuous dynamic systems, presented a framework based on hybrid optimal control, investigated existence and sensitivity results, introduced a modified stochastic search approach, and presented computational results for a tank changeover problem. Esposito and Floudas (2001) pointed out the theoretical rigor and advantages of the proposed global optimization methods by Esposito and Floudas (2000a) and the differences between local search approaches and global optimization methods. Esposito and Floudas (2002) studied the isothermal reactor network synthesis problem, formulated it as nonconvex NLP with differential-algebraic constraints, introduced a global optimization framework based on the integration approach and the αBB, investigated alternative types of reformulations, and reported extensive computational studies for complex reaction/reactor networks.

Banga et al. (2002) studied the optimal experimental design for the parameter estimation of nonlinear dynamic systems, formulated it as an optimal control that optimizes the Fischer information matrix, introduced two stochastic global optimization approaches to address the nonsmoothness and the multiplicity of solutions, and applied it to the parameter estimation of a fed-batch bioreactor. Papamichail and Adjiman (2002) introduced a deterministic spatial branch-and-bound global optimization approach for nonconvex models with ordinary differential equations, proposed a convex relaxation based on the theory of differential inequalities which allowed them to generate rigorous bounds for the parametric ODEs and their sensitivities, and applied their framework to small optimal control problems and reaction kinetics parameter estimation models. Adjiman and Papamichail (2003) developed further their branch-and-bound approach, proposed three convex relaxations for the parameter estimation of the initial value problem, and presented computational results on several parameter estimation problems in kinetics.

Singer and Barton (2003), Singer and Barton (2004) studied the global optimization of integral objective functions subject to ordinary differential equations, derived convex relaxations for the integral based on a pointwise integrand scheme, developed a branch-and-bound global optimization approach on a Euclidean space which combines the integrand convex relaxations with differential inequalities, McCormick's composition approach, and outer approximation, and illustrated their approach with several small benchmark problems. Lee and Barton (2003) studied the global optimization of linear time varying hybrid systems which exhibit both discrete state and continuous state behavior, and extended their recently developed approach for the determination of the optimal mode sequence when the transition times are fixed (Barton and Lee 2003), proposed a reformulation of the problem via binary variables while maintaining the linearity of the dynamical system, derived convex relaxations of Bolza-type functions using recent results for linear time varying continuous systems (Lee et al. 2004), and applied it to benchmark problems and an isothermal plug flow reactor problem.

Chachuat and Latifi (2003) introduced a spatial branch-and-bound global optimization approach for problems with ordinary differential equations in the constraints, presented results on the first and second order derivatives for the initial value problem and the two point boundary value problem, compared the sensitivity and the adjoint approaches, developed convex underestimators using the αBB principles, and presented computational studies and comparisons of the sensitivity versus the adjoint approach for several problems. Banga et al. (2003a) studied integrated process design and operation, parameter estimation in bioprocess models, and focused on stochastic global optimization methods for dynamic systems, addressed handling of constraints in stochastic methods, presented hybrid approaches for dynamic optimization, and presented computational studies on the optimal control of bioreactors, the integrated design of a waste treatment plant (see also Moles et al. (2003)) where they provided comparisons for several algorithmic approaches, and discussed advances in the parameter estimation of bioprocesses. Banga et al. (2003b) reviewed and introduced optimization as a key technology for food processing and discussed stochastic global optimization methods and their potential applicability in food process engineering.

Papamichail and Adjiman (2004) presented a deterministic spatial branch and bound global optimization algorithm for problems with a set of first-order differential equations in the constraints. They also presented a proof of convergence in a separate publication (Papamichail and Adjiman 2005). Barton and Lee (2004) presented a method for constructing convex relaxations of nonconvex NLPs with linear dynamic systems embedded. Chachuat et al. (2005) developed a decomposition approach for a general class of mixed-integer dynamic optimization problems that is capable of guaranteeing convergence to the global solution. They applied their method to the problem of optimal design and operation of a batch process consisting of a series reaction followed by a separation with no intermediate storage. Chachuat et al. (2006) presented an overview of global methods for dynamic programming, with emphasis on the control parameterization approach. Branch-and-bound algorithms for dynamic optimization are thoroughly discussed, and so is the outer-approximation algorithm for mixed-integer dynamic optimization problems. Future directions for research are proposed, and recently developed convex and concave relaxations for the solutions of nonlinear ODEs are also presented.

Barton et al. (2006) focused on the solution of optimization problems with continuous time automata embedded, and presented an overview of the control parameterization approach. They discussed the decomposition approach, restricted classes of subproblems such as the optimal mode sequences problem or the optimal transition times problem, and proposed future directions for research. Singer and Barton (2006) examined the global optimization of an integral objective function subject to nonlinear ordinary differential equations. They used McCormick's composition result to derive theory for the convex relaxation of an integral.

Lin and Stadtherr (2006, 2007) created a new interval solver for parametric ODEs, which is used to produce guaranteed bounds on the solution of dynamic systems with interval-valued parameters, and incorporated it within the framework of a global optimization solver for dynamic systems, including optimal control problems. They tested the new method on a collection of benchmark problems and reported more than an order of magnitude improvement in most cases. Long et al. (2006, 2007) applied a deterministic non-convex optimization method for nonlinear model predictive control of systems that exhibit nonlinear hybrid dynamics. They used discrete variables to model the multiple regimes of operation, and suggested some algorithm modifications to accelerate the solution of the resulting MINLP. Using a challenging wastewater treatment plant benchmark model, Egea et al. (2007b) conducted a computational comparison between various global optimization approaches, including surrogate-based methods. Egea et al. (2008) developed a new algorithm for the global optimization of costly nonlinear continuous problems. It is based on the scatter search metaheuristic (Egea et al. 2007a), which was coupled with a kriging-based prediction method in order to discard the evaluation of solutions that are not likely to provide high quality function values. Frits et al. (2007) used an interval arithmetic based branch and bound framework to find the singular points and bifurcations in studying feasibility of batch extractive distillation. Angira and Santosh (2007) applied the trigonometric differential evolution algorithm on dynamic optimization problems encountered in chemical engineering. They reported better computational performance when compared to the standard differential evolution algorithm, particularly in problems involving a large number of control stages.

5 Semi-infinite programming

Goberna and Lopez (2002) presented a review on the theoretical advances in linear and convex semi-infinite programming. In this section, we will focus on semi-infinite programming (SIP) from a global optimization perspective.

Levitin and Tichatschke (1998) considered a nonconvex generalized semi-infinite programming problem that involves parametric max-functions in both the objective and the constraints. They described conditions that ensure the uniform boundedness of the optimal sets of the dual problems with respect to the parameters, and developed a branch-and-bound approach that transform the global optimization problem into a finite series of convex problems. Liu and Teo (2002) considered quadratic SIP problems with positive definite objective and multiple linear infinite constraints. They proved that, just as in the case of single infinite constraints, the minimum parameterization number is less or equal than the SIP dimension. Moreover, they proposed an adaptive dual parameterization algorithm, proved its convergence, and presented numerical examples to demonstrate its improved efficiency compared to previous algorithms. Their algorithm was further improved by Liu et al. (2004) that presented a variant where, in each iteration, only a quadratic problem with a limited dimension and number of constraints is required to be solved.

Zakovic and Rustem (2003) considered solving a minimization SIP problem through a two stage procedure that searches for global maximum violation of the constraints. They also considered a version that searches for any violation of the constraints, and performed a computational comparison between the two variants. They applied these algorithms on various minimax (with or without coupled constraints) problems, as well as a small process design problem. Geletu and Hoffmann (2004) outlined theoretical considerations for determining coarse approximations of a solution of a generalized semi-infinite programming problem via global optimization of an exact discontinuous penalty approach. They extended the theory of robust analysis of marginal functions so as to study the behavior of the marginal functional of a resulting auxiliary parametric SIP problem.

Bhattacharjee et al. (2005a) used interval analysis methods to construct a finite reformulation of a semi-infinite program. This reformulation is generally over constrained relatively to the original SIP and, therefore, its solution constitutes a feasible upper bound to the SIP solution. This bound can be further refined by a subdivision procedure that was shown to converge to the true solution within finite epsilon. Bhattacharjee et al. (2005b) presented a branch and bound based deterministic global optimization algorithm for semi-infinite programs. The upper bounds are generated by replacing the infinite number of real-valued constraints with a finite number of constrained inclusion bounds, while the lower ones are generated via convex relaxations of a discretized approximation to the original problem. Chang and Sahinidis (2005) studied the optimization of metabolic pathways under stability considerations.

Their formulation is a bilevel optimization problem which they solve after transforming it to a semi-infinite optimization problem.

Floudas and Stein (2007) presented a novel adaptive convexification algorithm for the solution of semi-infinite optimization problems. The method adaptively constructs convex relaxations of the lower level problem based on αBB underestimators, replaces the relaxations with their equivalent KKT conditions, and solves the resulting mathematical programs with complementarity constraints. Liu (2007) presented a homotopy interior point method for globally solving semi-infinite programs. Mitsos et al. (2008a) considered nonconvex SIP problems and calculated relaxation-based bounds. They obtained lower bounds by solving a mathematical program with equilibrium constraints that resulted from discretization of the parameter set and KKT analysis of the lower-level maximization problem. Convex and linear relaxations of the latter were used for upper bounding.

6 Grey-box and nonfactorable models

Jones et al. (1998) introduced a response surface methodology, showed how the approximating functions can be used to construct an efficient global optimization algorithm, and addressed the computational difficulties that arise when solving auxiliary problems to balance the accuracy of the calculations with the computational performance. Byrne and Bogle (2000) studied the global optimization of modular flowsheeting systems, introduced an approach to modular based process simulation which is based on interval analysis and which can generate interval bounds, derivatives and their bounds for generic input–output modules, proposed a branch-and-bound global optimization algorithm, and applied it to an acyclic problem, and flowsheet with recycle. Jones (2001) provided a comparative overview of the various response surface approaches, with regard to their use in global optimization.

Gutmann (2001) introduced a global optimization method for problems where function evaluations are very expensive. The method relies on radial basis interpolation to define a utility function that is used to determine the next candidate point. Convergence was proved for various types of radial basis functions. Meyer et al. (2002) studied the global optimization of problems with nonfactorable constraints for which there does not exist an analytical form, proposed a sampling phase in which the nonfactorable functions and their gradients are sampled and a new blending function is constructed, and presented a global optimization phase in which linear underestimators and overestimators are derived via interval analysis and the interpolants are used as surrogates in a branch-and-cut global optimization algorithm. They also discussed a local optimization stage where the global optimum solution of the interpolation problem becomes the starting point for optimizing locally the original problem, and illustrated their approach through a small benchmark problem, an oilshale pyrolysis problem, and a nonlinear continuous stirred tank reactor model.

Sherali and Ganesan (2003) presented a pseudo-global optimization approach to address black-box problems. Their method utilizes a branch and bound framework where the lower bounds are calculated from response surface-generated polynomial approximations. The authors developed two alternative branching procedures and applied their methods in a containership design problem. Regis and Shoemaker (2005) proposed strategies that improve the performance of the radial basis function method of Gutmann (2001). They also presented a new approach for the constrained global optimization of expensive black box functions using response surface models (Regis and Shoemaker 2007). Huang et al. (2006) proposed a new global optimization method for stochastic black-box systems that is based on sequential kriging meta-models. A kriging based method was also developed by Davis and Ierapetritou

(2007, 2008) for the solution of NLPs and MINLPs containing black-box functions. Hu et al. (2007) presented a model reference adaptive search for global optimization.

7 Bilevel nonlinear optimization

Gümüş and Floudas (2001) studied the global optimization of bilevel nonlinear programming problems which involve twice continuously differentiable functions, proposed a convex relaxation of the inner problem followed by its equivalent representation via necessary and sufficient optimality conditions, introduced the αBB global optimization principles, presented a branch-and-bound framework, and applied it to several benchmark problems and parameter estimation problems. Floudas et al. (2001) introduced a global optimization approach for the calculation of the flexibility index and the feasibility test which are bilevel nonlinear optimization models, and demonstrated its applicability to a heat exchanger network problem, a pump and pipe run problem, a reactor-cooler system, and a prototype process flowsheet model.

Pistikopoulos et al. (2003) studied bilevel optimization models which are of linear–linear, linear–quadratic, quadratic–linear, or quadratic–quadratic type, and introduced approaches from parametric programming to transform the bilevel problem into a family of single level optimization problems which can be solved to global optimality, and presented computational results on several small benchmark problems. De Saboia et al. (2004) conducted a computational study of two global algorithms for linear bilevel programming and proposed some modifications that improve their computational performance. Ryu et al. (2004) addressed a bilevel decision-making problem under uncertainty in the context of enterprise-wide supply chain optimization with one level corresponding to a plant planning problem, while the other to a distribution network problem. The proposed strategy transforms the bilevel problem into a family of single parametric optimization problems that can be solved to global optimality.

Gümüş and Floudas (2005) studied the global optimization of bilevel mixed-integer optimization problems, proposed an approach that is applicable to mixed-integer nonlinear outer problem and twice continuously differentiable nonlinear inner problem, introduced another approach based on the convex hull representation of the inner problem, which is applicable when the inner level problem features functions which are mixed integer nonlinear in the outer variables and linear, polynomial, or multilinear in the inner integer variables, and linear in inner continuous variables; and applied it to several challenging benchmark problems.

Campelo and Scheimberg (2005) studied the linear bilevel problem and derived the characterization of a strict local solution. Babahadda and Gadhi (2006) used the notion of convexificator to establish necessary optimality conditions for bilevel optimization problems. Solodov (2007) considered the bilevel problem of minimizing a nonsmooth convex function over the set of minimizers of another nonsmooth convex function, and developed a bundle-type algorithm for solving it. Tuy et al. (2007) extended their monotonic optimization approach to handle general bilevel programming problems. They showed how the latter can be transformed into monotonic programs that can be solved by either polyblock approximation or branch-reduce-and-bound methods using monotonicity cuts. Faisca et al. (2007) proposed a global optimization approach for bilevel programming that is based on reformulating the inner optimization problem as a multi-parametric one, where the parameters are the variables of the outer level problem. They used their approach to solve quadratic, linear, and mixed-integer linear bilevel problems, with or without the presence of uncertainty. Mitsos et al. (2008b) developed a global optimization algorithm for bilevel problems with nonconvexities in both the inner and outer programs, presented a KKT-based heuristic for tightening of the lower bounds, extended the method to include branching, and analyzed two branching heuristics.

8 Summary

This paper reviewed the advances in global optimization during the period 1998–2008. The focal point was novel theoretical, algorithmic, and applications oriented advances on deterministic global optimization methods for (i) general twice differentiable NLPs; (ii) mixed-integer nonlinear optimization problems MINLPs; (iii) models with differential-algebraic constraints; (iv) grey-box and nonfactorable models; (v) semi-infinite programming problems; and (vi) bilevel nonlinear optimization problems.

From a computational point of view, the last decade witnessed significant advances. The expected technological advancement of computing machines, in conjunction with the introduction of novel approaches and application-targeted algorithms, has made possible the global optimization of larger and commercially more interesting problems. Recently, there have been several success stories that address medium to large scale problems. These include, representatively, the global optimization of: a multiproduct batch plant under uncertain demands (Harding and Floudas 1997), an NLP problem with 15,636 variables and about the same number of nonconvex terms of the type $xexp(y)$; a generalized pooling problem (Meyer and Floudas 2006), an MINLP formulation with 55 binary variables, 52 continuous variables, and nonconvexities that appear in the form of 156 distinct bilinear terms; a groundwater remediation network (Bringas et al. 2007), a simplified version of which amounted to an NLP formulation with 133 variables and 110 constraints that include 114 bilinear terms; and an integrated water network (Karuppiah and Grossmann 2008a), an MINLP consisting of 77 binary variables, 1,222 continuous variables, and 1,377 constraints that include 522 different bilinear terms.

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