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Global optimization in the 21st century: Advances and challenges

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Abstract

This paper presents an overview of the research progress in global optimization during the last 5 years (1998–2003), and a brief account of our recent research contributions. The review part covers the areas of (a) twice continuously differentiable nonlinear optimization, (b) mixed-integer nonlinear optimization, (c) optimization with differential-algebraic models, (d) optimization with grey-box/black-box/nonfactorable models, and (e) bilevel nonlinear optimization. Our research contributions part focuses on (i) improved convex underestimation approaches that include convex envelope results for multilinear functions, convex relaxation results for trigonometric functions, and a piecewise quadratic convex underestimator for twice continuously differentiable functions, and (ii) the recently proposed novel generalized αBB framework. Computational studies will illustrate the potential of these advances.

Keywords: Global optimization; Nonlinear optimization; Mixed-integer nonlinear optimization; Differential-algebraic optimization; Optimization with nonfactorable/grey-box models; Bilevel nonlinear optimization; Nonconvexities; Convex envelopes; Convex underestimators; Trilinear monomials; Trigonometric functions; Twice continuously differentiable functions

1. Introduction

It is now established that global optimization has ubiquitous applications not only in chemical engineering but also across all branches of engineering, applied sciences, and sciences (e.g., see the textbook by Floudas (2000a)). As a result, we have experienced significant interest in new theoretical advances, algorithmic and implementation related investigations, and their application to important scientific problems. A review paper discussed the advances in deterministic global optimization and their applications in the design and control of chemical process systems (Floudas, 2000b). A second review paper presented at the FOCAPD-1999 meeting outlined the chemical engineering research contributions in global optimization for the period 1994–1999, presented the advances, and identified research opportunities and challenges (Floudas & Pardalos, 1999). During the last 5 years, 1998–2003, several outstanding textbooks have been published addressing different facets of global optimization. These include the textbooks by Bard (1998), Floudas (2000a), Horst, Pardalos, and Thoai (2000), Sherali and Adams (1999), Tawarmalani and Sahinidis (2002), Tuy (1998) and Zabinsky (2003). A handbook of test problems in local and global optimization (Floudas et al., 1999), as well as two edited volumes of the research contributions presented at the major conferences on global optimization held in 1999 and 2003 (Floudas and Pardalos, 1999, 2003) were published. A recent survey paper by Neumaier (2004) discusses constrained global optimization and continuous constraint satisfaction problems with a particular emphasis on the use of interval arithmetic for addressing rounding off errors and reliability issues.

Global optimization addresses the computation and characterization of global optima (i.e., minima and maxima) of nonconvex functions constrained in a specified domain. Given an objective function f that is to be minimized and a set of equality and inequality constraints S, *Deterministic Global Optimization* focuses on the following important issues :

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(a) determine a global minimum of the objective function *f* (i.e., *f* has the lowest possible value in *S*) subject to the set of constraints *S*;
(b) determine *lower* and *upper bounds* on the global minimum of the objective function *f* on *S* that are valid for the whole feasible region *S*;
(c) determine an ensemble of qood quality local solutions in the vicinity of the global solution;
(d) enclose all solutions of the set of equality and inequality constraints *S*;
(e) prove that a constrained nonlinear problem is feasible or infeasible.

In this review paper, we will discuss the deterministic global optimization advances during the last 5 years 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) grey-box and nonfactorable problems, and (v) bilevel nonlinear and mixed integer optimization. We will first present all the contributions in the aforementioned classes, and we will subsequently focus on a few advances from Princeton University on (a) convex envelope results for trilinear monomials, (b) convex relaxation results for trigonometric functions, (c) new convex underestimators based on piecewise convex quadratic representations, and (d) the generalized αBB global optimization approach.

2. Twice continuously differentiable NLPs

In the first part of this section, we will review the advances in convex envelopes and convexification techniques. We will subsequently focus on theoretical and algorithmic advances for (a) general C^2 NLPs, (b) concave, bilinear, fractional, and multiplicative problems, (c) phase equilibrium problems, and (d) parameter estimation problems.

2.1. Convexification techniques and convex envelopes

Adjiman, Dallwig, Floudas, and Neumaier (1998a)and Hertz, Adjiman, and Floudas (1999) proposed several new rigorous methods for the calculation of the α parameters for (i) uniform diagonal shift of the Hessian matrix and (ii) nonuniform diagonal shift of the Hessian matrix, and they established their potential trade-offs. Adjiman, Androulakis, and Floudas (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.

Tawarmalani and Sahinidis (2001) developed the convex envelope and concave envelope for x/y over a unit hypercube, compared it to the convex relaxation proposed by Zamora and Grossmann (1998a, 1998b, 1999), proposed a semidefinite relaxation of x/y, and suggested convex envelopes for functions of the form $f(x)y^2$ and $f(x)/y$. 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, Ahmed, and Sahinidis (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 (2002) 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. Tawarmalani, Ahmed, and Sahinidis (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.

Liberti and Pantelides (2003) proposed a nonlinear continuous and differentiable convex envelope for monomials of odd degree, derived its linear relaxation, and compared to other relaxation. Björk, Lindberg, and Westerlund (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.

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. Meyer and Floudas (2004) presented explicit expressions for the facets of convex and concave envelopes of trilinear monomials with 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.

Caratzoulas and Floudas (2005) proposed novel convex underestimators for trigonometric functions which are trigonometric functions themselves. Akrotirianakis and Floudas (2005) 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. Meyer and Floudas (2004) 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.