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FULL LENGTH PAPER

A hybrid LP/NLP paradigm for global optimization relaxations

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Abstract Polyhedral relaxations have been incorporated in a variety of solvers for the global optimization of mixed-integer nonlinear programs. Currently, these relaxations constitute the dominant approach in global optimization practice. In this paper, we introduce a new relaxation paradigm for global optimization. The proposed framework combines polyhedral and convex nonlinear relaxations, along with fail-safe techniques, convexity identification at each node of the branch-and-bound tree, and learning strategies for automatically selecting and switching between polyhedral and nonlinear relaxations and among different local search algorithms in different parts of the search tree. We report computational experiments with the proposed methodology on widely-used test problem collections from the literature, including 369 problems from GlobalLib, 250 problems from MINLPLib, 980 problems from PrincetonLib, and 142 problems from IBMLib. Results show that incorporating the proposed techniques in the BARON software leads to significant reductions in execution time, and increases by 30% the number of problems that are solvable to global optimality within 500 s on a standard workstation.

Keywords Global optimization · Polyhedral relaxations · Nonlinear relaxations · Automatic convexity detection · Branch-and-reduce

Mathematics Subject Classification 90C11 · 90C25 · 90C26 · 90C57

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1 Introduction

Research in global optimization has witnessed a significant growth at the algorithmic and software levels over the last few years. Several general-purpose deterministic global solvers have been developed for nonconvex nonlinear programs (NLPs) and mixed-integer nonlinear programs (MINLPs), and are maturing rapidly. Beginning with the appearance of BARON in the mid 1990s [43], the following branch-and-bound based global solvers were introduced in the past decade: GlobSol [31], LindoGlobal [33], Couenne [7], SCIP [22], and ANTIGONE [35]. Performance of these algorithms is highly dependent on an effective use of state-of-the-art solvers for linear programming (LP), mixed-integer programming (MIP), and convex programming, at various stages in the global search (see [45] for an exposition).

Branch-and-bound algorithms rely on relaxations of nonconvex problems over successively refined partitions of the feasible region. That is, at each node in the search tree, in order to compute a bound on the optimal value of the original problem over the corresponding partition element, a relaxation of the nonconvex problem is constructed and optimized by a suitable optimization solver. Various relaxation construction techniques for nonconvex problems have been proposed in the literature. These methods can be broadly categorized as nonlinear convex relaxations [33,42], polyhedral relaxations [7,46,47], and piece-wise linear approximations [5,6]. Computational results reported over the past two decades demonstrate that, in comparison to LP solvers, local NLP solvers are slower and more susceptible to failure due to numerical difficulties. Motivated by this observation, Tawarmalani and Sahinidis [46] proposed the first branch-and-bound global optimization algorithm based on polyhedral relaxations. Using a factorable reformulation of the problem as the starting point, each univariate convex function was outer-approximated by its supporting hyperplanes at a number of carefully selected points. The authors found that while polyhedral relaxations introduce larger relaxation gaps compared to the convex relaxations from which they are derived, the superior performance and robustness of LP solvers significantly improves the reliability of LP relaxation-based global solvers. In a subsequent paper [47], Tawarmalani and Sahinidis addressed the question of constructing polyhedral relaxations for multivariate convex functions, and presented a branch-and-cut framework for global optimization of nonconvex NLPs and MINLPs based on the solution of LP relaxations. Furthermore, these authors showed that their proposed recursive polyhedral relaxations automatically exploit the convexity of intermediate expressions whose convexity follows from a recursive application of a set of well-known convexity preserving operations on a number of primitive functions. Due to its remarkable computational success, their proposed branch-and-cut framework was later adopted by other global solvers, currently including Couenne, GlobSol, SCIP, and ANTIGONE.

In this paper, we introduce a new relaxation paradigm for global optimization by combining polyhedral and convex nonlinear relaxations. In Sect. 2, we revisit the question of constructing strong polyhedral relaxations for nonconvex problems. We take the polyhedral relaxation framework of [47] as the starting point, and enhance and refine it in several directions. We strengthen the existing relaxations by generating supporting hyperplanes for intermediate convex expressions whose convexity is not implied by factorable composition rules. In addition, we improve the reliability of the

relaxation constructor in BARON by devising a cut generation scheme that examines the quality of the solution returned by the LP solver prior to utilizing it in global search.

In Sect. 3, we consider the case in which the continuous relaxation of a possibly nonconvex problems at a given node in the search tree is a convex optimization problem. Examples include convex NLPs, convex MINLPs, and nonconvex problems that become convex as a result of branching or range reduction operations. Current general-purpose global solvers based on LP relaxations employ a branch-and-cut algorithm even when the original problem is convex. While such an approach is quite stable and efficient for small problems, it is often significantly slower than solving NLP relaxations with gradient-based algorithms. We present a hybrid lower bounding scheme that combines polyhedral and nonlinear convex relaxations to make the most of state-of-the-art LP and convex NLP solvers. The main components of our implementation are (i) an efficient convexity detection tool that is embedded at every node in the branch-and-bound tree, (ii) a dynamic local solver selection strategy that can switch among various local solvers in the search tree based on their performance, (iii) a verification routine that examines the optimality of the solution returned by a local solver, and (iv) a hybrid relaxation constructor that alternates between polyhedral and nonlinear relaxations at every node based on their relative quality and numerical stability.

In Sect. 4, we present computational experiments on a variety of NLPs and MINLPs taken from GlobalLib [27], MINLPLib [11], PrincetonLib [40], and IBMLib [13]. Results show that the enhanced polyhedral relaxations and hybrid linear/nonlinear lower bounding scheme significantly improve the performance of BARON. In addition, a systematic comparison with a number of other solvers indicates the superiority of BARON 16 on a wide range of problem types. Finally, conclusions are offered in Sect. 5.

2 Polyhedral branch-and-cut

In this section, we consider the problem of constructing polyhedral relaxations for general nonconvex factorable programs. We first present some preliminary material on factorable programming relaxations as well as the outer-approximation method proposed in [47]. Subsequently, we discuss strengths and weaknesses of the existing framework and propose several enhancements.

2.1 Factorable programming and polyhedral relaxations

Factorable programming relaxations [34] have formed the basis of currently popular techniques in global optimization for bounding nonconvex functions. A variant of this technique introduced by Ryoo and Sahinidis [42] starts by iteratively decomposing a nonconvex factorable function, through introduction of auxiliary variables and constraints for intermediate expressions, until all intermediate expressions can be outer-approximated by a convex feasible set. That is, each nonlinear factorable expression in the problem formulation is replaced by a collection of equality constraints, each of which has the form $t = f(x)$, where t denotes an auxiliary variable and $f(x)$ is an intermediate expression. Current implementations of factorable relaxations

in general-purpose global solvers [7,22,33,35,44] employ this nested decomposition to the extent that all intermediates are affine functions, univariate convex (concave) functions, bilinear expressions, or other functions whose convex/concave envelopes are known. Subsequently, the nonconvex set defined by each intermediate equation is outer-approximated by a convex set. In particular, if $f(x)$ is a bilinear function, then $t = f(x)$ is replaced by two inequalities $t \geq \check{f}(x)$ and $t \leq \hat{f}(x)$, where $\check{f}(x)$ and $\hat{f}(x)$ denote the polyhedral convex and concave envelopes of $f(x)$, respectively. Alternatively, if $f(x)$ is a univariate convex (resp. concave) function, then $t = f(x)$ is replaced by $t \leq \hat{f}(x)$ and $t \geq f(x)$ (resp. $t \leq f(x)$ and $t \geq \check{f}(x)$), where the affine function $\hat{f}(x)$ (resp. $\check{f}(x)$) denotes the concave envelope (resp. convex envelope) of $f(x)$ (see [46] for further details). The resulting optimization problem is nonlinear and convex, possibly with many more variables than the original nonconvex problem, and its solution provides a lower bound for the optimal value of the original minimization problem.

To capitalize on the availability of highly efficient LP solvers, in [46], the authors proposed the use of entirely polyhedral relaxations by further underestimating (resp. overestimating) each convex (resp. concave) univariate via supporting hyperplanes at a number of points determined by a sandwich algorithm. The resulting LP is solved at each node in the branch-and-bound tree to generate a lower bound. This methodology was further refined in [47], where at each node additional cutting planes are generated in rounds and added to the polyhedral relaxation only if they violate the relaxation solution. In general, the nested factorable decomposition and relaxation may introduce a large relaxation gap. In [47], the authors showed that the proposed factorable relaxation framework automatically exploits the convexity of original functions, under certain assumptions. In the following, we briefly describe this result in a slightly different form (see also Theorem 1 in [47]). First, we recall a convexity-preserving operation, which is a powerful tool for detecting convexity of a wide class of functions (see Section 3.2 in [10] for more details).

Lemma 1 *Let $f : \mathcal{D} \to \mathbb{R}^n$ be a vector of functions f_j, $j \in J = \{1, \ldots, n\}$, where $\mathcal{D} \subset \mathbb{R}^m$ is a convex set. Let $\bar{J}$ contain the elements of J for which f_j is not affine. Assume that f_j is convex for $j \in J_1 \subseteq \bar{J}$ and concave for $j \in J_2 = \bar{J} \setminus J_1$. Let $g : \mathcal{C} \to \mathbb{R}$ be convex, where $\mathcal{C}$ is a convex set in $\mathbb{R}^n$ that contains the range of all f_j over $\mathcal{D}$. Assume that $g(y_1, \ldots, y_n)$ is nondecreasing in y_j, $j \in J_1$ and is nonincreasing in y_j, $j \in J_2$. Then, the composite function $h(x) = g(f(x))$ is convex on $\mathcal{D}$.*

Various well-known convexity-preserving operations follow from the above result. For instance, if $f_j, j \in J$ are affine functions, then it follows that convexity is preserved under the affine mapping of the domain. Similarly, if we restrict g to be a univariate convex function, then Lemma 1 simplifies to the following composition rule: a convex nondecreasing (resp. nonincreasing) function of a convex (resp. concave) function is convex.

Now, consider a factorable decomposition of $h(x) = g(f(x))$ defined as $y_j = f_j(x)$ for all $j \in J$, and $z = g(y)$. For simplicity, let f and g be differentiable and let f denote a vector of convex functions, i.e., $J = J_1$. Suppose that convexity of $f(x)$ and $g(y)$ are recognizable by the relaxation constructor, whereas convexity of

$h(x)$ is not known a priori. Our goal is to generate a polyhedral underestimator for z at $(x, y) = (x_0, y_0)$, where $y_0 = f(x_0)$. By convexity and monotonicity assumptions on f and g, a factorable relaxation of z is given by $y_j \geq f_j(x_0) + \nabla f_j(x_0)^T (x - x_0)$ for all $j \in J$ and $z \geq g(y_0) + \nabla g(y_0)^T (y - y_0)$. By assumption, $g(y)$ is componentwise nondecreasing. Thus, $z \geq g(y_0) + (\nabla f(x_0)^T \nabla g(y_0))^T (x - x_0)$, where $\nabla f(x_0)$ denotes the jacobian of $f(x)$ at $x = x_0$. By the chain rule of differentiation, $\nabla h(x_0) = \nabla f(x_0)^T \nabla g(y_0)$. Therefore, $z \geq h(x_0) + \nabla h(x_0)^T (x - x_0)$, i.e., recursive relaxation automatically exploits the convexity of $h(x)$, in the sense that its projection onto the space of original variables corresponds to the supporting hyperplane of $h(x)$ at $x = x_0$.

In the remainder of the paper, by *primitive functions*, we refer to the set of functions whose convexity properties are recognizable by a factorable relaxation scheme. Moreover, we will refer to those convexity-preserving operations that are implied by Lemma 1, as *composition rules*. Hence, the above discussion implies that recursive factorable relaxations automatically exploit convexity of functions whose convexity can be described by a recursive application of composition rules on a set of primitive functions.

2.2 Exploiting convexity for cut generation

There exist several classes of functions whose convexity are not exploited by the conventional factorable relaxation scheme. For instance, in BARON's factorable programming module, the list of primitive functions consist of affine expressions, monomials (x^a), powers (a^x), logarithmic functions, bilinears, and fractions. As a result, to generate a convex outer-approximation of the set $\mathcal{P} = \{(x, f) : f = x \log x, x \in [0.1, 1]\}$, a decomposed equivalent of f is constructed as follows: $y = \log x$, $f = xy$. Subsequently, to obtain a convex relaxation of $\mathcal{P}$, the nonconvex set defined by each equation is replaced by its convex hull. It is then simple to show that the projection of this convex relaxation onto the original space (x, f) is given by:

$$\mathcal{S} = \{(x, f) : \max\{-2.05x - 0.03, 2.56(x - 1.0)\} \leq f \leq \log x/10\}.$$

The set $\mathcal{S}$ is depicted in Fig. 1a, where it can be seen that the recursive relaxation introduces a large relaxation gap. As a second example, in Fig. 1b, a factorable relaxation of $\mathcal{P} = \{(x, f) : f = \sqrt{1 + x^2}, -0.5 \leq x \leq 2.0\}$ is shown. It is simple to verify that the function $f = \sqrt{1 + x^2}$ is convex. However, as a composite function, f is a concave increasing function ($f = \sqrt{y}$) of a convex function ($y = 1 + x^2$), a structure that does not satisfy the assumptions of Lemma 1.

Motivated by the above discussion, we present several important classes of functions whose convexity or concavity are *not* exploited by the conventional factorable approach. Clearly, our list is by no means complete, and there exist many convex functions that we do not consider in our implementation. However, the following list is based upon an extensive survey of a large number of optimization problems that appear in widely-used test libraries as well as a variety of applications. We state these results without proofs, as the proofs follow from elementary arguments.

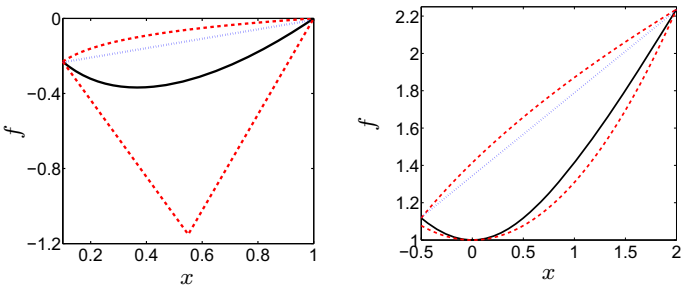


Fig. 1 Conventional factorable relaxations for functions whose convexity do not follow from composition rules. The convex function f is shown in solid black and its factorable outer-approximation is shown in dashed red. In both figures, the dotted blue line is the concave envelope of f. **a** $f = x \log x$, $0.1 \leq x \leq 1.0$, **b** $f = \sqrt{1 + x^2}$, $-0.5 \leq x \leq 2.0$ (colour figure online)

1. *Products and ratios.* Consider the function

$$f(x) = \prod_{i \in I} f_i(x_i), \ I = \{1, \ldots, n\}, \ n \geq 2,$$

where $f_i = x_i^{a_i}$, $a_i \in R \setminus \{0\}$ or $f_i = a_i^{x_i}$, $a_i > 0$ for all $i \in I$. Then, $f(x)$ is convex if one of the following conditions is satisfied:
(i) $f_i = a_i^{x_i}$, or $f_i = x_i^{a_i}$ with $x_i > 0$, $a_i < 0$ for all $i \in I$.
(ii) $f_i = x_i^{a_i}$ with $x_i > 0$, $a_i < 0$ for all $i \in I \setminus \{j\}$, for some $j \in I$, and $f_j = x_j^{a_j}$ with $a_j > 1$, $f_j \geq 0$ and $\sum_{i \in I} a_i \geq 1$.
Moreover, $f(x) = \prod_{i \in I} x_i^{a_i}$ is concave if $a_i > 0$ for all $i \in I$ and $\sum_{i \in I} a_i \leq 1$.
2. *Perspective of functions.* The perspective operation preserves convexity, i.e., if $f(x)$ is convex, then its perspective $g(x, y) = yf(x/y)$, $y > 0$ is jointly convex in x and y (see Section 3.2.6 in [10]). Examples include perspective of negative entropy $g = x \log(x/y)$, and perspective of exponential $g = y \exp(x/y)$.
3. *Norms and norm-type functions.* Consider the function

$$f(x) = \left(a_0 + \sum_{i=1}^{n} a_i x_i^p \right)^q, \ x \in \mathbb{R}^n, \ p, q \in \mathbb{R}, \ n \geq 1,$$

where $a_i > 0$, $i = 0, 1, \ldots, n$. Then, $f(x)$ is convex if one of the following conditions is satisfied:
(i) $p > 1$, $q < 1$, and $pq \geq 1$; e.g. $f = \sqrt{x_1^2 + x_2^2}$
(ii) $p < 0$, and $0 < q < 1$; e.g. $f = \sqrt{1 + 1/x}$.
Moreover, $f(x)$ is concave if $p < 1$, $0 < pq < 1$, and $p(q - 1) > 0$; e.g. $f = (1 + \sqrt{x})^2$.
4. *Quadratic functions and quadratic norms.* Consider the function $f(x) = x^T Q x$, $x \in \mathbb{R}^n$, $Q \in \mathcal{S}^n$, where $\mathcal{S}^n$ denotes the set of $n \times n$ symmetric matrices. Then, $f(x)$ is convex (resp. concave) if and only if Q is positive semidefinite (resp. negative semidefinite). Moreover, the Q-quadratic norm (resp. seminorm) defined

as $||x||_Q = \sqrt{x^T Qx}$, where Q is positive definite (resp. positive semidefinite), is a convex function.

5. *Log-sum-exp* The function $f = \log(c_0 + c_1 a_1^{x_1} + \cdots + c_n a_n^{x_n})$, where $x \in \mathbb{R}^n$ and $c_i > 0$ for $i = 0, \ldots, n$ is convex.
6. *Negative entropy* $f = x \log x$, $x > 0$ is a convex function.

Remark 1 It is possible to construct many more types of convex functions by applying composition rules to the functions listed above. However, there is no need to characterize all such functions. A factorable relaxation automatically exploits such structures, provided that the above functions are included in the list of primitive functions of the factorable scheme. For example, consider $h(x) = (\prod_{i=1}^n f_i(x))^{1/n}$, $x \in \mathbb{R}^m$. Suppose that f_i, $i = 1, \ldots, n$ are concave and nonnegative. The geometric mean $g(y) = (\prod_{i=1}^n y_i)^{1/n}$, $y_i \geq 0$ belongs to Class 1 above, and thus is concave. In addition, $g(y)$ is nondecreasing in each argument. Hence, by Lemma 1, $h(x)$ is concave, and its concavity is automatically exploited by the recursive relaxation.

Remark 2 Consider the set $\mathcal{S} = \{(x, f) : f = x_1\sqrt{1 + (\log x_2)^2}, x \in [\underline{x}, \bar{x}]\}$, and suppose that the goal is to obtain a convex relaxation of $\mathcal{S}$. Clearly, as a function of x, f does not belong to any type of functions listed above. A factorable reformulation of this set is given by $\mathcal{S}' = \{(x, y, f) : y_1 = \log x_2, y_2 = y_1^2, y_3 = 1 + y_2, y_4 = \sqrt{y_3}, f = x_1 y_4, x \in [\underline{x}, \bar{x}]\}$. In the lifted space (x, y, f), we can deduce the relation $y_4 = \sqrt{1 + y_1^2}$, which, by Part (i) of Class 2, corresponds to the graph of a univariate convex function, and thus can be outer-approximated but its convex hull. It is important to note that, since factorable relaxations are already built in the lifted space, generating strong cuts for such intermediate relations can significantly enhance the convergence rate of a branch-and-bound algorithm.

Remark 3 To identify convex/concave quadratics, we decompose a quadratic function into nonseparable components and compute the eigenvalues of each quadratic form to detect its convexity. As we detail in the following, we store both eigenvalues and eigenvectors of quadratics to generate additional classes of cutting planes. Furthermore, for indefinite quadratic functions with non-polyhedral envelopes, we generate cutting planes based on the separable programming approach of [41]. In this paper, we do not consider quadratic forms with polyhedral envelopes as BARON is equipped with a powerful relaxation constructor for such functions [4].

Remark 4 Consider a second-order cone constraint defined as

$$\sum_{i=1}^{n} a_i x_i^2 - a_0 x_0^2 \leq 0, \; x_i \in \mathbb{R}, \; a_i > 0, \quad \forall i \in \{0, 1, \ldots, n\}. \tag{1}$$

Clearly, the quadratic function $f = \sum_{i=1}^n a_i x_i^2 - a_0 x_0^2$ is not convex. However, inequality (1) defines a convex set. It is simple to verify that the factorable relaxation of f do not exploit the convexity of this set. We reformulate constraints of the form (1) as

$$\left(\sum_{i=1}^{n} a_i x_i^2\right)^{0.5} - \sqrt{a_0} x_0 \leq 0. \tag{2}$$

Since l_2-norm belongs to Class 3 functions listed above, when applied to the left-hand side of inequality (2), the proposed factorable relaxation does not introduce any relaxation gap.

Remark 5 Consider the function $f = x_1^{0.3}x_2^{0.4}x_3^{0.5}$, $x \geq 0$. This function is not concave. However, if at least one of the variables get fixed, then the resulting function is concave. In addition, if two of the variables become fixed, then concavity of the resulting univariate function is exploited by the conventional factorable scheme. As another example, consider $f = x_1^3/\log x_2$, $x_1 \in \mathbb{R}$, $x_2 > 1$. This function is neither convex nor concave. However, if at some node in the search tree, as a result of an earlier branching or range reduction, we have $x_1 \geq 0$ (resp. $x_1 \leq 0$), then f becomes convex (resp. concave).

We employ the following two-step approach to generate tighter polyhedral relaxations at each node in the branch-and bound tree:

Recognition Prior to the initialization of the branch-and-bound tree, we mark and classify all intermediate relations containing subexpressions whose convexity/concavity cannot be exploited by the conventional factorable approach. Let us denote such intermediates by $y_j = f_j(x)$, $j \in J$. The data structures required for generating and storing cutting planes are also allocated at this stage.

Cut generation At each node in the branch-and-bound tree, we first construct and solve a crude outer-approximation of the problem based on the conventional factorable reformulation. Subsequently, various classes of cutting planes are generated and added to the current relaxation iteratively, only if they violate the relaxation solution (see [47] for details). We do not add the proposed cutting planes to the initial outer-approximation but utilize them for the iterative cut generation scheme. At a given cut generation iteration, we scan all expressions $y_j = f_j(x)$, $j \in J$ stored at the recognition step. Denote by (x^*, y_j^*) the projection of the current relaxation solution to the (x, y_j) space. If any of the variables are fixed in the current node, we eliminate them and update $f_j(x)$ accordingly. If $f_j(x)$ is a convex function (resp. concave function) that is not recognized as such by the conventional factorable scheme and $y_j^* < f_j(x^*)$ (resp. $y_j^* > f_j(x^*)$), then a cut of the form $\nabla f_j(x^*)^T x - y_j \leq \nabla f_j(x^*)^T x^* - f_j(x^*)$ (resp. $\geq$) is added to the current relaxation.

2.3 Exploiting convexity for domain reduction

In addition to generating cutting planes, detecting convexity of intermediate expressions may result in inferring tighter bounds for both original and auxiliary variables of a nonconvex problem. Given lower and upper bounds on original variables, factorable programming-based global solvers employ a recursive bound propagation scheme based on interval arithmetic and monotonicity analysis to infer bounds on all intermediate variables. Subsequently, in a backward mode, bounds on the objective and constraint functions are used to infer tighter bounds on original and intermediate variables. Clearly, if an intermediate relation is convex (resp. concave), then we can compute its minimum (resp. maximum) to obtain a sharp lower bound (resp. upper

bound) for the associated auxiliary variable. Accordingly, we tighten the bounds on all convex/concave intermediates, whenever such bounds are not implied by the existing bound propagation scheme. For instance, consider $f = x \log x$, $x \in [0.1, 2]$. By convexity of f, it follows that $f \in [-0.368, 1.386]$. However, in the recursive approach, we have $f = xy$, where $y = \log x$. Utilizing interval bounds for the bilinear term $f = xy$, $0.1 \le x \le 2$, $-2.3 \le y \le 0.69$, we obtain $f \in [-4.605, 1.386]$. Similarly, we exploit convexity (or concavity) of univariate quadratics of the form $ax^2 + bx$ to enhance the impact of feasibility-based bounds tightening operators (see [17] for details).

As another example, consider a nonseparable convex quadratic function $f = x^T Qx + b^T x$, $x \in \mathbb{R}^n$, $Q \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$, $n \ge 2$. In this case, we compute the minimum of f over $\mathbb{R}^n$ by solving a system of linear equations and use it to bound f in the relaxation. If f is unbounded below over $\mathbb{R}^n$, i.e., if b is not in the column space of Q, then we ignore the linear part of f and add the inequality $\sum_{1\le i\le j\le n} q_{ij} y_{ij} \ge 0$, where $y_{ij} = x_i x_j$ to the relaxation, as a zero lower bound on $x^T Qx$ is not inferred by existing bound propagation schemes in BARON. Now, suppose that a finite upper bound on f is available, i.e., $x^T Qx + b^T x \le \alpha$. The feasible region defined by this inequality is an ellipsoid (or a degenerate ellipsoid). In this case, we characterize the hyperplanes corresponding to the minimum-volume bounding box of this ellipsoid, and add them to the relaxation. For completeness, in the following, we present the derivation of these inequalities.

First, suppose that f does not contain any linear term. Denote by λ_i and v_i the ith eigenvalue and eigenvector of Q, respectively. By convexity of f, we have $\lambda_i \ge 0$ for all $i = 1, \ldots, n$. Without loss of generality, suppose that the first m eigenvalues of Q are positive. Clearly, if f is strictly convex, then $m = n$. It follows that $f = \sum_{i=1}^m \lambda_i (v_i^T x)^2$. By assumption, α is a finite upper bound on f. Thus, we obtain $2m$ inequalities given by $-\sqrt{\alpha/\lambda_i} \le v_i^T x \le \sqrt{\alpha/\lambda_i}$, for $i = 1, \ldots, m$. Now, suppose that f contains linear terms. As in the previous case, we would like to reformulate f as a sum of squares, i.e., we are interested in finding the vector $c \in \mathbb{R}^m$ such that $x^T Qx + b^T x = \sum_{i=1}^m \lambda_i (v_i^T x + c_i)^2 - \sum_{i=1}^m \lambda_i c_i^2$. After rearranging terms and using the relation $x^T Qx = \sum_{i=1}^m \lambda_i (v_i^T x)^2$, we obtain

$$\sum_{i=1}^{m} (\lambda_i v_{ij}) c_i = b_j/2, \quad \forall j = 1, \ldots, n, \tag{3}$$

where v_{ij} denotes the jth element of v_i. Two cases arise:

- The linear system (3) has a solution; clearly, if Q is positive definite, i.e., $m = n$, then the system always has a solution. In this case, the minimum-volume bounding box of the feasible region is given by the following inequalities:

$$-\sqrt{\frac{\alpha + \sum_{j=1}^m \lambda_j c_j^2}{\lambda_i}} - c_i \le v_i^T x \le \sqrt{\frac{\alpha + \sum_{j=1}^m \lambda_j c_j^2}{\lambda_i}} - c_i, \quad i = 1, \ldots, m.$$

- The linear system (3) does not have any solutions; if Q is positive semi-definite, then (3) has more equations than unknowns and may not have any solutions, i.e.,

the feasible region is an elliptic paraboloid. In this case, if a finite upper bound β on the quadratic form $x^T Qx$ is available, then we ignore the linear part of f and generate the bounding box of the region defined by $x^T Qx \leq \beta$.

2.4 Exploiting quasi-convexity for cut generation

Consider the set $\mathcal{S}$ defined as $\mathcal{S} = \{(x_1, x_2) \in \mathbb{R}^2 : x_1 \geq 0,\ x_1^2 x_2 \geq 1\}$. The function $f = x_1^2 x_2$, with $x_1 \geq 1$, $x_2 \in \mathbb{R}$ is neither convex nor concave. However, the set $\mathcal{S}$ is convex as it is a superlevel set of the quasi-concave function f. Recall that a function is quasiconcave if and only if all of its superlevel sets $\mathcal{S}_\alpha = \{x : f(x) \geq \alpha\}$, for $\alpha \in \mathbb{R}$ are convex (see [2] for an exposition). To generate supporting hyperplanes of $\mathcal{S}$, we first reformulate $x_1^2 x_2 \geq 1$ as $x_2 \geq 1/x_1^2$, and subsequently linearize the latter inequality using first-order Taylor series approximation of the convex function $1/x_1^2$. In general, it is always possible to represent sublevel sets of quasiconvex functions (or superlevel sets of quasiconcave functions) via inequalities of convex functions (see Section 3.4 in [10]).

To demonstrate the benefit of such reformulations for constructing tighter relaxations, in Fig. 2, we depict the factorable relaxation of $\mathcal{S}$ projected onto the original space. This relaxation is obtained by first reformulating $\mathcal{S}$ as $\bar{\mathcal{S}} = \{(x_1, x_2, y_1, y_2) : y_1 = x_1^2,\ y_2 = y_1 x_2,\ x_1 \geq 0,\ y_2 \geq 1\}$ and then replacing the nonconvex set defined by each equality constraint by its convex hull over the corresponding domain. To construct such a relaxation, finite lower and upper bounds on all variables are required. Hence, we assume $x_1 \in [0.1, 1]$, $x_2 \in [1, 100]$. Alternatively, a relaxation can be constructed by combining the two techniques, i.e., by reformulating $y_1 x_2 \geq 1$ as $x_2 \geq 1/y_1$, and employing the factorable relaxation of $y_1 = x_2^2$ as before. As can be seen in Fig. 2, while stronger than the pure factorable approach, the hybrid scheme is not tight. For this example, it is simple to show that if the exponent of x_1 is smaller than one, then the hybrid approach does not introduce any relaxation gap. In the following, we formalize this idea. First, we recall the conditions under which a signomial term is quasiconvex or quasiconcave (see Chapter 5 of [2] for proofs). Clearly, convexity is a sufficient condition for quasi-convexity. Since convex/concave signomials are covered by the techniques discussed in the previous section, we only consider cases in which f is quasiconvex (resp. quasi-concave) but is not convex (resp. concave). We refer to such functions as merely quasiconvex (resp. merely quasi-concave).

Lemma 2 *Consider the function* $f = \prod_{i \in I} x_i^{a_i}$, $a_i \in \mathbb{R} \setminus \{0\}$ *for all* $i \in I = \{1, \ldots, n\}$. *Define* $I_p = \{i \in I : a_i > 0\}$, *and* $I_n = I \setminus I_p$ *and* $\mathcal{C} = \{x \in \mathbb{R}^n : x_i \geq 0,\ \forall i \in I_p,\ x_i > 0,\ \forall i \in I_n\}$. *Then,* f *is merely quasiconcave over* $\mathcal{C}$ *if one of the following conditions is satisfied:*

(i) $a_i > 0$ *for all* $i \in I$, *and* $\sum_{i \in I} a_i > 1$,
(ii) $a_i > 0$ *for all* $i \in I \setminus \{j\}$ *for some* $j \in I$, *and* $\sum_{i \in I} a_i \leq 0$.

Moreover, f *is merely quasiconvex over* $\mathcal{C}$, *if* $a_i < 0$ *for all* $i \in I \setminus \{j\}$ *for some* $j \in I$, *and* $0 \leq \sum_{i \in I} a_i < 1$.

We now utilize the above result to construct tighter polyhedral relaxations for nonconvex problems that contain quasi-convex expressions. In the following, we assume

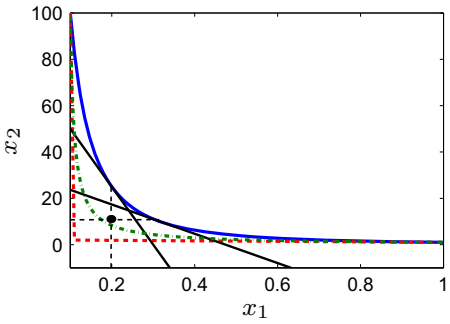


Fig. 2 Alternative relaxation methods for the set $\mathcal{S} = \{(x_1, x_2) : x_1^2 x_2 \geq 1, x_1 \in [0.1, 1], x_2 \in [1, 100]\}$. The boundary of set $\mathcal{S}$ is shown in solid blue, its factorable relaxation is shown in dashed red, and a hybrid relaxation is shown in dotted green. The two tangent lines show the cutting planes associated with two convex reformulations of $x_1^2 x_2 \geq 1$, i.e., (i) $1/x_1^2 - x_2 \leq 0$ and, (ii) $1/\sqrt{x_2} - x_1 \leq 0$, which separate the point $(x_1, x_2) = (0.2, 1.0)$ from the enlarged feasible regions (colour figure online)

that f is defined over a box $[\underline{x}, \bar{x}] \subset \mathcal{C}$, where the set $\mathcal{C}$ is defined in the statement of Lemma 2. In addition, by $\underline{f}$ and $\bar{f}$, we imply interval lower and upper bounds on $f(x)$, respectively, i.e., $\underline{f} = \prod_{i \in I_n} \bar{x}_i^{a_i} \prod_{i \in I_p} \underline{x}_i^{a_i}$ and $\bar{f} = \prod_{i \in I_n} \underline{x}_i^{a_i} \prod_{i \in I_p} \bar{x}_i^{a_i}$.

Lemma 3 *Consider the function $f(x)$, $x \in [\underline{x}, \bar{x}]$ defined in the statement of Lemma 2. Suppose that $y = f(x)$ is an intermediate relation introduced by the factorable reformulation of a nonconvex problem. Denote by $\underline{f}$ and $\bar{f}$ the interval bounds on $f(x)$, and let $\underline{y}$ and $\bar{y}$ denote lower and upper bounds on y, respectively. Suppose that $\underline{f} < \underline{y}$ or $\bar{y} < \bar{f}$. Denote by x^* the solution for a relaxation of the nonconvex problem. We have the following cases:*

(i) *if $f(x)$ is quasiconcave with $a_i > 0$ for all $i \in I$ and $f(x^*) < \underline{y}$, then an inequality of the form $l(x) - x_j \leq 0$ for some $j \in I$ cuts off the relaxation solution, where $l(x)$ is the supporting hyperplane of the convex function $z = \left(\prod_{i \in I \setminus \{j\}} x_i^{a_i} / \underline{y}\right)^{-1/a_j}$ at $x_i = x_i^*$ for all $i \in I \setminus \{j\}$.*

(ii) *if $f(x)$ is quasiconcave (resp. quasiconvex) with $a_j < 0$ (resp. $a_j > 0$) for some $j \in I$ and $f(x^*) < \underline{y}$ (resp. $f(x^*) > \bar{y}$), then the inequality $x_j - l(x) \leq 0$ cuts off the relaxation solution, where $l(x)$ is the supporting hyperplane of the concave function $z = \left(\prod_{i \in I \setminus \{j\}} x_i^{a_i} / \gamma\right)^{-1/a_j}$ at $x_i = x_i^*$ for all $i \in I \setminus \{j\}$, and $\gamma = \underline{y}$ (resp. $\gamma = \bar{y}$).*

Proof We state the proof for Part(i). The proof of Part(ii) follows from a similar line of arguments. Note that if $\underline{y} \leq \underline{f}$ and $\bar{f} \leq \bar{y}$, then the relation $\underline{y} \leq f(x) \leq \bar{y}$ is valid for all $x \in [\underline{x}, \bar{x}]$ and no useful cut can be generated. Now, suppose that $f(x^*) < \underline{y}$. Clearly, $\underline{y} > 0$. Hence $x_i > 0$ for all $i \in I$ at any point satisfying the inequality $f(x) \geq \underline{y}$. Consider $\prod_{i \in I} x_i^{a_i} \geq \underline{y}$. Since $a_i > 0$ and $x_i > 0$ for all $i \in I$, this inequality can be equivalently written as $(\prod_{i \in I \setminus \{j\}} x_i^{a_i} / \underline{y})^{-1/a_j} \leq x_j$ for any $j \in I$. It is simple to show that the signomial term on the left-hand side of this inequality is convex (see Part (ii) of Class 1 functions in Sect. 2.2), and thus replacing

it by a supporting hyperplane at $x = x^*$ results in a valid inequality that enforces $f(x^*) \geq \underline{y}$. □

In principle, the above reformulation technique can be used to generate cutting planes for any inequality of the form $f(x) \leq \underline{y}$, where f is a quasi-convex function. However, at this stage, our implementation is restricted to the case where f is either a signomial term or a function obtained by application of composition rules to signomials.

2.5 Safe lower bounds

At each node in the branch-and-bound tree, a global optimization solver constructs and solves polyhedral relaxations to obtain lower bounds on the optimal value of the nonconvex problem. For many problems, these LP relaxations are ill-conditioned and contain constraints with very large and/or very small coefficients. This issue often arises for nonconvex problems that contain unbounded variables or nonlinear expressions that are not properly bounded. While the state-of-the-art LP solvers are quite reliable, there exist cases for which these solvers make false optimality or infeasibility claims (see for example [39]). For instance, we have observed that LP solvers occasionally return a solution that violates a number of constraints by a small amount. As a result, the relaxation constructor generates identical (or very similar) cutting planes and adds them to the current relaxation. Subsequently, the solution returned by the LP solver remains unchanged, and the same set of cutting planes may be appended to the relaxation and sent to the LP solver for multiple rounds. As another example, for badly scaled LPs that are on the border of infeasibility, LP solvers tend to make false infeasibility claims. By simply accepting such false infeasibility claims and pruning the corresponding nodes, the global solver may fail to locate a global solution. To address these issues, we add cutting planes to the relaxation only if they are properly scaled. Additionally, we accept LP solver solutions only after verifying their optimality, and examine infeasibility certificates prior to pruning any node:

Safe cuts Consider a cutting plane of the form $\sum_{i \in I} a_i x_i \leq b$, where $a_i \in \mathbb{R} \setminus \{0\}$, for all $i \in I = \{1, \ldots, n\}$, $b \in \mathbb{R}$. To avoid a poorly scaled model, we add this cut to the LP relaxation if the following conditions are satisfied: (i) $l \leq |a_i| \leq u$ for all $i \in I$, (ii) $l \leq |a_i/a_j| \leq u$ for all $i, j \in I$ such that $i < j$, and (iii) $|b| \leq \bar{b}$. Here, the implementation-specific constant $l > 0$ is acceptably small, and $0 < u < \bar{b}$ are acceptably large.

To maintain the tightness of polyhedral relaxations, prior to the initial outer-approximation of each convex/concave univariate $f(x)$, $x \in \mathcal{C} \subseteq \mathbb{R}$, the algorithm locates an interval $\mathcal{L} \subseteq \mathcal{C}$, over which the resulting supporting hyperplanes satisfy the above conditions. Finally, prior to appending cutting planes to an existing relaxation, we scale the cuts so that our measure of violation agrees with the feasibility tolerance of the LP solver.

Safe LP bounds We verify the optimality of the primal-dual pair reported by the LP solver prior to utilizing them in the global search. In particular, we check for primal

feasibility, dual feasibility, and zero duality gap. We have observed many cases for which the solution returned by the LP solver is slightly infeasible. This issue often arises if the original nonconvex problem contains (many) nonlinear equality constraints or if the polyhedral relaxation is poorly scaled. For such instances, if the LP solution is dual feasible, then by weak duality, the dual objective value serves as a valid lower bound for the problem. LP solvers such as `CPLEX` and `CLP` provide Farkas certificates for infeasible models. Namely, if an infeasible LP has an unbounded dual, then finding a recession direction of the dual problem is sufficient to prove the infeasibility of the primal. Hence, to identify false infeasibility claims, we demand and examine the associated certificates.

3 Hybrid LP/NLP relaxation paradigm

Consider a convex optimization problem in standard form:

$$\begin{aligned} \text{(CV)} \qquad & \min_x \ f_0(x) \\ & \text{s.t.} \ \ f_i(x) \leq 0, \quad i = 1, \ldots, m \\ & \qquad Ax - b = 0, \end{aligned}$$

where $x \in \mathbb{R}^n$, $A \in \mathbb{R}^{p \times n}$, $b \in \mathbb{R}^p$, and $f_0, \ldots, f_m$ are convex functions. Various cutting plane-based algorithms have been proposed for solving convex NLPs by solving a sequence of LPs [8,32]. These methods are used mostly for solving non-smooth convex problems or large-scale structured convex problems such as nonlinear network flows. For general smooth convex problems, however, methods based on active sets or interior point algorithms are often significantly faster, even though they are more prone to numerical difficulties. Because of such difficulties, for some convex problems, state-of-the-art local solvers report sub-optimal solutions or make false infeasibility claims. It is well-known that for differentiable convex problems, every primal-dual pair that satisfies the KKT conditions is optimal. Therefore, a practical approach to solve convex problems could first utilize local NLP solvers and, if these solvers fail due to numerical issues, then the algorithm could utilize the more stable but slower polyhedral-based techniques.

In the context of global optimization, convex subproblems often appear as a result of relaxing or restricting the feasible region of the original nonconvex problem at various stages during the global search. For example, convex subproblems are obtained by relaxing integrality requirements in convex MINLPs or restricting the domain of a subset of variables in nonconvex NLPs, as a result of applying range reduction or branching operations. Clearly, an extreme yet important case is when the original NLP is convex. Global solvers such as `SCIP`, `LindoGlobal` and `ANTIGONE` detect convexity of quadratic programs (QPs) and quadratically constrained quadratic programs (QCQPs) prior to the initialization of the branch-and-bound tree, and solve convex problems with local solvers. For more general problem classes, prior to the initialization of the branch-and-bound tree, `SCIP` employs a symbolic approach to detect the convexity of each constraint function $g(x) \leq 0$ in the problem formula-

tion. If convexity of $g(x)$ is verified, no factorable reformulation of this constraint is required and the corresponding convex feasible region is outerapproximated by supporting hyperplanes in the course of the branch-and-bound tree (see Section 7.3 of [48] for details). However, current general-purpose global solvers are not equipped with automatic convexity detection facilities at every node of the branch-and-bound tree, and utilize the conventional branch-and-bound algorithm to solve non-quadratic convex subproblems as well.

Motivated by the above discussion, in this section, we introduce a hybrid lower-bounding paradigm that aims to harness the advantages of both polyhedral and nonlinear convex relaxations by combining them in a dynamic fashion. The main components of our implementation are (i) an efficient convexity detection tool that checks if the continuous relaxation of the problem is convex at every node in the branch-and-bound tree, (ii) a dynamic local solver selection strategy that switches among various local solvers in the branch-and-bound tree based on their performance, (iii) an examiner that verifies if the solution returned by the local solver is optimal, and (iv) a hybrid relaxation constructor that alternates between polyhedral and nonlinear relaxations at every node based on their relative strength and numerical robustness. We detail each of these components below.

3.1 Automatic convexity detection

To expedite the global search, we embed an efficient convexity detector at every node in the branch-and-bound tree. As we describe in the following, our convexity verification approach is based on a number of basic principles of convex analysis, which have also been implemented in other computational environments [21,28]. The main distinction between our method and earlier convexity assessment techniques stems from the different contexts in which the results of such analysis are utilized. Our starting point is a highly efficient polyhedral-based branch-and-cut framework, and our goal is to improve the global solver by exploiting convexity of subproblems at every node in the branch-and-bound tree. Clearly, such an approach is only beneficial if convexity verification can be conducted very fast; for instance, by performing all expensive computations at the root node. In the following, we briefly review existing automated convexity assessment techniques, and subsequently describe our implementation.

3.1.1 Background

Due to its significant theoretical and algorithmic implications, assessing convexity properties of general optimization problems in a fully automated manner is of great interest. The problem of determining whether or not a general optimization problem is convex is NP-hard [1]. Nevertheless, several incomplete techniques have been proposed in the literature that can effectively prove or disprove convexity of many practical optimization problems. These approaches can be categorized in two main groups:

Symbolic methods These techniques are based on the following observation. Given a set of primitive functions whose convexity and monotonicity properties are known a priori, and a set of convexity-preserving operations, we can construct many more convex functions via a recursive application of these operations on the primitive set. Similarly, given a general nonlinear function, we can utilize this technique to possibly verify its convexity. This approach was introduced by Grant et al. [29] for constructing convex optimization problems called disciplined convex programs (DCP). The authors also developed the modelling framework `CVX` to support the DCP methodology [28]. The `CVX` system verifies if the input problem is a valid DCP, converts it to a solvable form and sends it to a solver. This symbolic technique was later adopted by Fourer et al. [20] to verify the convexity of a given optimization problem. The resulting implementation is available as part of `DrAmpl` [21], a meta solver for analyzing structural properties of optimization problems including convexity. The main advantage of the symbolic approach is its low computational cost. However, it may fail to prove or disprove convexity for many cases, an outcome we will henceforth call *inconclusive*.

Numerical methods Several techniques have been proposed to prove or disprove convexity of a given problem by verifying various properties of convex functions. Given a multivariate function, `MProbe` [12] checks the basic definition of convexity over randomly generated line segments in the feasible region. Clearly, this approach can only be used for disproving convexity. In `DrAmpl` [21], if the symbolic approach described above returns an inconclusive flag, then the algorithm proceeds to the numerical disproving phase in which it tries to find a direction of negative curvature by solving an auxiliary quadratic program. Nenov et al. [38] assess convexity by checking positive semi-definiteness of interval Hessians, an approach which in spite of generality is often quite expensive. In [36], the author proposes an efficient method to compute the bounds on eigenvalues of interval Hessians.

3.1.2 Convexity detection for global optimization

Our convexity detection technique is based on the symbolic approach with the exception of quadratic functions for which we check if the Hessian is positive semidefinite. In other words, we include quadratic functions in the list of primitive functions, and utilize a numerical approach to verify their convexity. We will further detail our convexity detection algorithm for quadratics in the next section. In addition, our convexity-preserving ruleset consists of any operation implied by Lemma 1. For a given ruleset, generality of the symbolic detection approach depends on the list of primitive functions. As we described in Sect. 2, to generate sharp factorable-based polyhedral relaxations, we have enhanced the list of `BARON`'s primitive functions by including a variety of convex/concave functions that appear in applications. We utilize the same list of functions for our convexity detector.

To assess convexity of a general nonlinear function, we start from its factorable reformulation and associate the set of intermediate relations with a recursive application of composition rules on a number of primitive functions. In addition, to determine convexity and monotonicity of primitive functions, we make use of `BARON`'s bound propagation facilities. We illustrate this technique by a simple example and refer the

reader to [3,20,28] for a detailed description of the symbolic convexity verification scheme. Consider the inequality constraint $(x_1^2 + x_2^2 + 1)^2 \leq 4$, $x \in \mathbb{R}^2$. A factorable reformulation of this constraint is given by $y_1 = x_1^2$, $y_2 = x_2^2$, $y_3 = y_1 + y_2 + 1$, $y_4 = y_3^2$, $y_4 \leq 4$. Using interval arithmetic, BARON infers the following bounds: $x \in [-1, 1]^2$, $(y_1, y_2) \in [0, 1]^2$, $y_3 \in [1, 2]$, $y_4 \in [1, 4]$. To assess convexity properties of this constraint, we first identify convexity and monotonicity of all intermediate relations in the *lifted space*: (i) $y_1 = x_1^2$ and $y_2 = x_2^2$ are convex; since y_1 and y_2 are functions of x variables, no monotonicity analysis is required for these functions, (ii) $y_3 = y_1 + y_2 + 1$ is affine and nondecreasing in each argument, (iii) $y_4 = y_3^2$ is convex and increasing over $y_3 \in [1, 2]$. Next, we employ convexity-preserving operations to deduce convexity in the *original space*: (i) $y_3 = y_1 + y_2 + 1$ is affine and nondecreasing in both arguments, and y_1 and y_2 are convex functions of x; thus, by Lemma 1, y_3 is a convex function of x, (ii) y_4 is a convex increasing function of y_3, and y_3 is a convex function of x; again, by Lemma 1, y_4 is a convex function of x, implying convexity of the original inequality constraint.

It is important to note that BARON's range reduction strategies are highly important for our convexity detection scheme as they utilize the feasible region of the original problem to infer tighter bounds for variables. For example, consider the function $f = (x_1 - x_2)^3$, $x \in [0, 1]^2$ with a factorable reformulation given by $y = x_1 - x_2$, $f = y^3$, $y \in [-1, 1]$. Clearly, $f(x)$ is nonconvex over the unit hypercube. Now, assume that we have an additional constraint of the form $x_1 \geq x_2$ in the model. Using this inequality, BARON infers $y \in [0, 1]$. Then, it follows that f is a convex increasing function of an affine function, and is therefore convex.

We embed our convexity detection technique in BARON's preprocessor as well as every node in the branch-and-reduce algorithm. Our ultimate goal is to reduce the overall execution time of the global solver for a wide range of optimization problems. Hence, a highly efficient convexity verification algorithm is of crucial importance. Otherwise, the detection algorithm may deteriorate the performance of the global solver, specially for problems with a large number of nonconvex sub-problems in the branch-and-bound tree. The main steps of our convexity detection algorithm are outlined next.

Reformulation Prior to the application of convexity detector, we utilize a number of simple transformations that are beneficial for the purpose of convexity assessment:

(i) $\log(a^x)$ is replaced by $x \log a$,
(ii) $a^{\log x}$ is replaced by $x^{\log a}$,
(iii) $(x^a)^b$ is replaced by x^{ab} with the exception of non-differentiable functions (see Sect. 2.5),
(iv) $(a^x)^b$ is replaced by $(a^b)^x$,
(v) $(x_1 \dots x_n)^a$ is replaced by $x_1^a \dots x_n^a$,
(vi) quadratic functions are converted into an expanded form: (1) all products are disaggregated, i.e., $x_0(a_0 + a_1x_1 + \cdots + a_nx_n)$ is replaced by $a_0x_0 + a_1x_0x_1 + \cdots + a_nx_0x_n$; a similar reformulation is employed for the more general form $(a_0 + a_1x_1 + \cdots + a_nx_n)(b_0 + b_1y_1 + \cdots + b_ny_n)$, (2) monomials of the form $(a_0 + a_1x_1 + \cdots a_nx_n)^2$ are expanded only if such a reformulation is needed for

convexity detection. Namely, the monomial is expanded, if one of the following two conditions is satisfied: (i) if in the same constraint, there exists a bilinear term which has a common variable with the monomial; e.g. the inequality $(x_1+x_2)^2 - 2x_1x_2 \leq 1$ is replaced by the inequality $x_1^2+x_2^2 \leq 1$, (ii) if in the same constraint, there exists another monomial whose coefficient has the opposite sign and the two monomials have common variables; e.g. the inequality $(x_1+2x_2)^2+x_1^2-2x_2^2 \leq 1$ is replaced by the inequality $2x_1^2 + 4x_1x_2 + 2x_2^2 \leq 1$.

For instance, consider the reformulation (i) above. As a composite function, the function $f = \log(a^x)$ is a concave increasing function (log) of a convex function (a^x), a case whose convexity or concavity does not follow from Lemma 1. However, in the reformulated form, $f = x \log a$ is clearly an affine function. The above operations are applied in a recursive manner until we obtain a formulation for which none of these operations are applicable. For example $f = \sqrt{2^{\log(x+y)}}$ simplifies to $f = (x+y)^{\log\sqrt{2}}$ by first replacing $2^{\log(x+y)}$ by $(x+y)^{\log 2}$ using rule (ii) and subsequently replacing $((x+y)^{\log 2})^{0.5}$ by $(x+y)^{\log\sqrt{2}}$ using rule (iii).

Initial convexity assessment With the objective of minimizing the overall computational cost of convexity detection, prior to the initialization of the branch-and-bound tree, we mark all convex expressions in the problem, identify various sources of nonconvexity, and store the information for later investigation. In particular, we classify variables that contribute to the nonconvexity of the problem as follows. Consider an optimization problem whose convexity is verifiable by the proposed detection scheme only if a subset of (original) variables become fixed. We refer to this subset as the set of *nonconvex variables*. For example, consider the constraint $x_1^2+\log x_2 \leq 1$; in this case, x_2 is a nonconvex variable, whereas, for the constraint $x_1^2+\log(x_1+2x_2) \leq 1$, both x_1 and x_2 are marked as nonconvex variables. Now, consider the function $f = (x_1-2x_2)^3$, $x \in \mathbb{R}^2$. Clearly, f is neither convex nor concave. However, if at some node in the branch-and-bound tree, we have $x_1 - 2x_2 \geq 0$ (resp. $x_1 - 2x_2 \leq 0$), then f is convex (resp. concave) in that node. Note that according to the conventional factorable reformulation, an auxiliary variables y is defined as $y = x_1 - 2x_2$. Hence, if at a node in the branch-and-bound tree, the lower bound on y is nonnegative (resp. nonpositive), we conclude that $x_1 - 2x_2 \geq 0$ (resp. $x_1 - 2x_2 \leq 0$). Accordingly, we define a *concavoconvex variable* as an original variable or as an auxiliary variable that is an affine combination of original variables appearing in concavoconvex monomials, i.e., $f = x^{2k+1}$, $k = 1, 2, \ldots$, $x \in [\underline{x}, \bar{x}]$ such that $\underline{x} < 0 < \bar{x}$. In addition, with each concavoconvex variable x_j (or $y_j = a^T x + b$), we associate a domain restriction flag η_j, defined as: (i) $\eta_j = 1$, if x_j appears in concavoconvex monomials with positive coefficients, in which case the problem is convex only if x_j takes nonnegative values, (i) $\eta_j = -1$, if x_j appears in concavoconvex monomials with negative coefficients; in this case, if the problem becomes convex, then we have $x_j \leq 0$ and, (iii) $\eta_j = 0$, if x_j appears in concavoconvex monomials with positive and negative coefficients; in this case, if x_j takes nonzero values then the problem is nonconvex. We should remark that each variable can appear in at most one of the above lists based on the following dominance relations: (i) if a variable appears in concavoconvex terms with $\eta_j = 1$ (or $\eta_j = -1$), and nonconvex terms, then we append it to the list of nonconvex vari-

ables, (ii) if a variable appears in concavoconvex terms with $\eta_j = 0$ and nonconvex terms, then we mark it as a concavoconvex variable with $\eta_j = 0$. In the following, we describe the procedure for initial convexity assessment of a general factorable NLP.

Consider a constraint of the form $h_1(x_1) + \cdots + h_m(x_m) \leq \alpha$, $m \geq 1$, $x \in [\underline{x}, \bar{x}] \subseteq \mathbb{R}^n$, where each $h_j(x_j)$ is a primitive function or a composition of primitive functions, $x_j \in \mathbb{R}^{n_j}$, $n_j \leq n$ contains some components of x, $\alpha \in \mathbb{R}$ is a scalar, and $h_j(x_j)$ cannot be represented as $h_j = \sum_{k=1}^{K} h_{jk}$, where each h_{jk} is a primitive function (or a composition of primitive functions). For example, consider the constraint $x_1^2 + 1.5(x_1 \log x_1)^2 + x_2^2 + 2x_1x_2 - \exp(-x_2^2) \leq 1$ with $h_1(x_1, x_2) = x_1^2 + 2x_1x_2 + x_2^2$, $h_2(x_1) = 1.5(x_1 \log x_1)^2$, and $h_3(x_2) = -\exp(-x_2^2)$. In this case, we do not further decompose h_1 to square and bilinear terms, as a nonseparable quadratic function belongs to the list of primitive functions. In addition, a decomposition of the form $h_2 = 1.5(x_1 \log x_1)^2 - \exp(-x_2^2)$ is not valid, since this expression is not a primitive function, and can be decomposed into two subfunctions $h_{21} = 1.5(x_1 \log x_1)^2$ and $h_{22} = -\exp(-x_2^2)$, each of which is obtained by an application of composition rules to primitive functions. First, suppose that $h_j(x_j)$ is not a quadratic function containing bilinear terms. We associate a *convexity flag* ω_j with each $h_j(x_j)$, defined as follows:

(i) $\omega_j = 1$: the convexity detector verifies convexity of $h_j(x_j)$. We mark this function as convex, and do not re-examine its convexity in subsequent nodes.

(ii) $\omega_j = -1$: the convexity detector either verifies concavity of $h_j(x_j)$ or returns an inconclusive flag that is unchangeable unless all variables in $h_j(x_j)$ become fixed. In this case, we append x_j to the list of nonconvex variables, and do not revisit h_j later in the search tree. For example, consider $f = \log(x_1^2 + x_2^2 + 1)$. As a composite function, f is a concave increasing function of a (strictly) convex function; a structure that is not covered by Lemma 1, and will not change during the search tree unless both x_1 and x_2 are fixed.

(iii) $\omega_j = 0$: the convexity detector returns an inconclusive flag; however, convexity properties of h_j may change later, as a result of range reduction or branching operations. In this case, h_j is marked for later check in the branch-and-bound tree. Moreover, if $h_j = (c^T x_j + d)^{2k+1}$, $k = 1, 2, \ldots$ is concavoconvex, then we append $y = c^T x_j + d$ to the list of concavoconvex variables. For example, consider $f = (x_1^2 - x_2)^2$, $x \in [-1, 1]^2$. In this case, f is a convex nonmonotone function of a convex function, which is an inconclusive composition. In fact, it is simple to verify that, over $[-1, 1]^2$, the function f is neither convex nor concave. However, if at some node in the search tree x_1 is fixed or the lower bound of the auxiliary variable y_2 defined as $y_2 = y_1 - x_2$, where $y_1 = x_1^2$ is nonnegative, then convexity of f is verifiable by the proposed detection scheme.

Now, suppose that $h_j(x_j)$ is a nonseparable quadratic function containing bilinear terms. For notational simplicity, we drop the subscript j from x_j in the following. To assess convexity properties of $h_j(x) = x^T Q x = \sum_{i=1}^{n} \sum_{k=1}^{n} q_{ik} x_i x_k$, we first check the sign of first- and second-order principal minors of Q. Namely, (i) if h_j contains a square term x_i^2 with a negative coefficient, then we append x_i to the list of nonconvex variables, (ii) for any bilinear term $x_i x_k$ in h_j with $q_{ii} \geq 0$ and $q_{kk} \geq 0$, if $q_{ii} q_{kk} - q_{ik}^2 < 0$, then we add $x_i x_k$ to the list of *nonconvex bilinears*, i.e., if h_j is

convex at a certain node, then either x_i or x_k is fixed. Subsequently, we classify h_j as follows:

(i) if all square terms in h_j have negative coefficients, then h_j does not become convex unless all x variables are fixed. In this case, we let $\omega_j = -1$, and do not revisit h_j later in the search tree.
(ii) if Q has at least one negative first- or second-order principal minor, then we let $\omega_j = 0$, and mark h_j for later check in subsequent nodes.
(iii) if all first- and second-order principal minors of Q are nonnegative, then we compute its eigenvalues. If all eigenvalues of Q are nonnegative, we mark h_j as convex, i.e., $\omega_j = 1$; otherwise, we let $\omega_j = 0$, and utilize the following criterion to determine whether it is necessary to recalculate eigenvalues of the Hessian in descendent nodes:

Lemma 4 *Consider a quadratic function $h(x) = x^T Qx$, $x \in \mathbb{R}^n$. Suppose that Q has p negative eigenvalues. Let $h(\tilde{x})$ denote a convex quadratic function obtained by fixing a subset of variables in $h(x)$. Then, $h(\tilde{x})$ has at most $n - p$ variables.*

Proof Suppose that $h(\tilde{x})$ has $n - p + 1$ variables and, without loss of generality, assume that $h(\tilde{x})$ is obtained by fixing the last $p - 1$ components in x, i.e., $\tilde{x} = [x_1, \ldots, x_{n-p+1}]$. Denote by $\mathcal{S}$ the subspace spanned by all $\tilde{x} \in \mathbb{R}^{n-p+1}$. Let $V = \{v^i\}_{i=1}^n$ denote a set of n orthonormal eigenvectors of Q, and let $V' = \{v^{i_1}, \ldots v^{i_p}\}$ be the set eigenvectors associated with negative eigenvalues (λ) of Q. Denote by $\mathcal{T}$ the p-dimensional subspace spanned by the eigenvectors in V'. It follows that $\mathcal{S} \cap \mathcal{T}$ contains at least one nonzero vector of the form $u = \sum_{j \in J} \alpha_j v^j$, $J = \{i_1, \ldots, i_p\}$, $\alpha \in \mathbb{R}^p$. By orthonormality of the vectors in V', it follows that $h(u) = u^T Qu = \sum_{j \in J} \lambda_j \alpha_j^2 < 0$, which is in contradiction with the assumption that the restriction of $h(x)$ to $\mathcal{S}$ is convex. Thus, $h(\tilde{x})$ has at most $n - p$ variables. □

Therefore, for each nonconvex quadratic h_j with nonnegative first- and second-order principal minors, we store the number of negative eigenvalues p_j, and re-examine positive-semidefiniteness of the Hessian only if at least p_j variables in h_j are fixed. A similar procedure is applied for convexity assessment of quadratic forms that are composed with other nonlinear functions.

The techniques outlined above are utilized in the first call to the convexity detector during BARON's preprocessor. Subsequently, at the root node, we update the initial assessment, if applicable. For instance, if at the root node a nonconvex variable is fixed or a concavoconvex variable has the proper domain, then they are removed from the corresponding lists. The purpose of such updates is to minimize the computational cost of convexity detection in subsequent nodes in the branch-and-bound tree. Clearly, if during the initial assessment or at the root node it turns out that $\omega_j = 1$ for all j, then the problem is convex, and the detection algorithm terminates.

Early termination tests Consider a bilinear program (P), i.e., the problem of minimizing a bilinear function subject to bilinear inequality constraints. Clearly, P becomes convex if and only if, for every bilinear term $x_i x_j$ in the formulation, at least one of x_i and x_j is fixed to a certain value. In other words, problem (P) is convex only when it

reduces to an LP. The same argument holds for QCQPs consisting of component-wise concave quadratic functions. Clearly, for these examples, the global solver does not benefit from convexity detection. In general, we would like to identify cases for which convexity detection is not useful so as to avoid the extra computational cost in the branch-and-bound tree.

At every call to the convexity detector, we first mark all fixed variables and eliminate them from the factorable reformulation of the optimization problem. More precisely, we call $x_i \in [\underline{x}_i, \bar{x}_i]$, a fixed variable, if $\bar{x}_i - \underline{x}_i \leq \epsilon$, for some $\epsilon > 0$.

Denote by n_f the number of (original) variables that are fixed at the current node. Subsequently, we mark all variables that appear linearly in the problem; let n_l denote the number of such variables. Define $n_r = n - n_f - n_l$, where n is the number of variables in the original problem. Clearly, if $n_r = 0$, then this problem is an LP and the convexity detector terminates. Let n_c denote the number of nonconvex variables and denote by n_o the number of original concavoconvex variables with $\eta = 0$, at the current node. It follows that, if $n_r = n_c + n_o$, then the convexity detector is not beneficial as the problem remains nonconvex unless all variables that appear in nonlinear expressions become fixed. In particular, if this equality holds during preprocessing or at the root node, then the convexity detector will be deactivated for this problem.

Fast convexity detection strategies At every node in the branch-and-bound tree, we utilize the information stored during the initial convexity assessment to speed up the convexity detector. We start by examining the list of nonconvex and concavoconvex variables. If a nonconvex variable is not fixed in this node or a concavoconvex variable does not have the proper domain, then the problem is still nonconvex and the convexity detector terminates. For problems containing multivariate quadratic expressions, we employ the following tests: (i) if a nonconvex bilinear term is not linear in this node or, (ii) if a quadratic function with n variables and k negative eigenvalues has more than $n - k$ unfixed variables, then the problem is still nonconvex. If the above conditions do not disprove the problem's convexity, we proceed to the next step and scan the list of nonlinear expressions with $\omega_j = 0$, as defined in Step II. If convexity of any of the functions is not verifiable or a function is found to be nonconvex, then the convexity detector terminates. Otherwise, the problem is marked as convex in this node.

Finally, since convexity of QCQPs does not depend on variable bounds, we define a list of *convexity patterns* $\mathcal{L}_C = \{l^k\}_{k \in K}$ for this problem class. Namely, once convexity of the QCQP is verified at a given node, we append the index set of fixed variables $\tilde{l}$ to the list of convexity patterns. In addition, we keep the size of $\mathcal{L}_C$ minimal by removing any l^k from the list that is implied by $\tilde{l}$. In subsequent nodes, prior to the utilization of convexity detection tests, we compare the index set of fixed variables l^0 with those stored in $\mathcal{L}_C$ and, if $l^0 \supseteq l^k$ for any $k \in K$, we conclude that the problem is convex.

With the exception of quadratic functions, our convexity detection tool relies on an efficient use of symbolic operations. In general, existing numerical verification algorithms are too expensive to be embedded in the branch-and-bound tree. However, an interesting possibility would involve utilizing the numerical approach of [36] to examine convexity properties of certain types of functions for which the symbolic test is inconclusive.

3.2 Dynamic local solver selection

Once convexity of the continuous relaxation of a sub-problem is verified at a given node in the branch-and-bound tree, we employ a local solver to compute a lower bound by solving the convex NLP. Hence, a highly efficient and reliable local solver is key to the success of this approach. Through our experiments with several state-of-the-art local solvers, we have observed that each solver behaves quite differently on various problem types and, more importantly, there is no single solver that outperforms others on a wide range of optimization problems. In fact, even for a single problem in the course of the branch-and-bound tree, as the global solver searches through different parts of the feasible region, the most suitable local solver may vary. Consequently, to maximize the impact of convexity detection and increase the likelihood of finding better upper bounds on the global solution, we devised a dynamic local solver selection scheme that alternates among various solvers based on their performance in the branch-and-bound tree.

Suppose that we have access to a number of local solvers for the global search. Prior to the application of each local search in the branch-and-bound tree, we would like to employ a simple algorithm that selects a solver with the highest chance of success. To measure the success rate of a local solver, we associate a binary flag *win* with each call to that solver defined as follows: (i) for upper bounding, the local solver wins ($win = 1$), if it returns a solution that passes our feasibility test and improves the value of the best known upper bound, (ii) for lower bounding, the local solver wins ($win = 1$), if it returns a solution that satisfies the KKT conditions. We store this information as follows: for each solver, we store (i) the total number of wins in the branch-and-bound tree denoted by N_{wins} and (ii) the number of consecutive wins/losses denoted by N_{gains}, where a positive number for N_{gains} indicates the number of consecutive wins, whereas a negative number corresponds to the number of consecutive losses. Furthermore, if m consecutive wins (resp. losses), are followed by a loss (resp. win), then N_{gains} is reset to zero. Finally, we define a rank $r_s \in [1, \bar{r}]$ for each solver s. At a given node, solvers are selected for local search based on this rank. A smaller value for rank implies a higher chance of success. We initialize the rank of each solver based on our prior knowledge regarding solver average performance on a large number of test problems, and update r_s during the global search as follows. If a solver fails η consecutive times, then we decrease the frequency at which the solver is called by downgrading its rank: $r_s = \min(2r_s, \bar{r})$. Similarly, if a solver wins η consecutive times, we upgrade its rank using the relation $r_s = \max(1, r_s/2)$. Prior to each local search, we employ the above learning procedure to select a local solver as follows. If all local solvers have failed too often, i.e., $r_s = \bar{r}$ for all solvers, then the solver with the largest total number of wins (N_{wins}) is selected; otherwise, a solver with the best rank is utilized for local search.

3.3 Combining polyhedral and nonlinear relaxations

Suppose that the input problem is an NLP. If its convexity is verified during preprocessing or at the root node, then as soon as a local solver returns a solution that satisfies

the KKT conditions, BARON terminates. To avoid branching for convex problems, at the root node, we utilize all available local solvers based on their rank, and proceed to the branching step only if they all fail to find an optimal solution. In the following, we describe the integration of nonlinear relaxations into BARON's branch-and-cut framework.

Suppose that the convexity detector verifies that a sub-problem in the branch-and-bound tree is convex. We select a local solver from the list of available solvers using the dynamic scheme outlined in the previous section. It is well known that even for convex problems, a good starting point can highly affect the performance of local solvers. Indeed, providing a near-optimal starting point often expedites the convergence rate of Newton-type methods significantly. We construct a crude polyhedral relaxation of the convex NLP using BARON's polyhedral relaxation constructor and utilize its solution as the starting point for the local solver. If the solution reported by the local solver satisfies the KKT conditions, then the optimal value of the convex NLP is used as the lower bound in this node; otherwise, the local solver's solution is discarded and BARON continues with the conventional polyhedral relaxation scheme as detailed in [47]. In addition, to avoid the extra cost of solving many NLPs for which the local solver fails to find an optimal solution, we adjust the frequency at which the NLP lower bounding scheme is used based on the performance of local solvers.

Now, consider the case where the primal-dual pair $(\tilde{x}, \tilde{\nu})$ returned by the local solver is not optimal but is dual feasible, i.e., the gradient of the Lagrangian with respect to x vanishes at $(\tilde{x}, \tilde{\nu})$. By weak duality, the value of the Lagrangian $L(x, \nu)$ at $(\tilde{x}, \tilde{\nu})$ serves as a lower bound to the optimal value of the convex NLP. In this case, we set the lower bound to $LB = \max(L(\tilde{x}, \tilde{\nu}), \hat{f})$, where $\hat{f}$ is the lower bound obtained by BARON's polyhedral relaxation constructor.

Finally, if both the LP and NLP solvers fail, we resort to calculating a simple interval extension of the objective function in order to obtain a lower bound for the current node. Clearly, the parent node bound is valid for the children. We use the strongest available bound for each node to ensure bound monotonicity. Subsequently, we proceed to branching by bisecting the longest edge so as to guarantee convergence. Moreover, if an earlier LP was successfully solved for the node, we revert to the solution of that LP before branching.

In this paper, we make use of local NLP solvers for lower bounding only if the continuous relaxation of the original problem is convex at the current node. More generally, local NLP solvers can be utilized to optimize nonlinear factorable relaxations of nonconvex problems of the type considered in [42]. However, these relaxations often have many more variables and constraints compared to the original problem and are more prone to solver failures. Designing efficient hybrid schemes for optimizing these nonlinear factorable relaxations is a subject of future research.

4 Numerical experiments

The purpose of this section is to demonstrate the computational benefits of the proposed techniques by incorporating them in the branch-and-reduce global solver BARON

[43,47]. To this end, we consider a variety of NLPs and MINLPs from widely-used collections of test problems: 980 NLPs from `PrincetonLib` [40], 369 NLPs from `GlobalLib` [27], 250 MINLPs from `MINLPLib` [11], and 142 MINLPs from `IBMLib` [13]. These test sets were obtained after eliminating problems involving trigonometrics, error functions and other expressions that `BARON` cannot handle from the original collections. In Table 1, we provide some statistics on the size of the problems used in our computations in terms of the numbers of constraints (m), variables (n), discrete variables (n_d), nonzero elements in the constraints and objective (nz), and nonlinear nonzero elements in the constraints and objective (nnz). Each test set contains a wide range of nonlinear problems, ranging from univariate optimization problems to problems with more than 20,000 variables, most of which have a significant nonlinear component.

Throughout this section, all experiments are performed with `GAMS 24.7.2` on a 64-bit Intel Xeon X5650 2.66 GHz processor; all implementations are single-threaded. In addition, all problems are solved with relative/absolute optimality tolerance of 10^{-6}, and a CPU time limit of 500 s. Other algorithmic parameters are set to the default settings of the `GAMS` distribution for all solvers. When comparing the performance of different algorithms, we call a problem trivial if all algorithms take less than half a second to solve it to optimality. Denote by $f_{p,s}$, $s \in \mathcal{S}$ the feasible solution returned by solver s upon termination for model p, and let f_p^* denote the best feasible solution among all solvers, i.e., $f_p^* = \min_{s\in\mathcal{S}} f_{p,s}$. To measure the relative quality of the solution returned by each algorithm, we define

$$\Delta_{p,s} = \begin{cases} f_{p,s} - f_p^*, & \text{if } |f_p^*| < 1, \\ (f_{p,s} - f_p^*)/|f_p^*|, & \text{otherwise.} \end{cases} \tag{4}$$

In particular, we say that solver s finds the best solution for problem p, if $\Delta_{p,s} < 10^{-3}$. In addition, we say that problem p is solved to global optimality by global solver s, if (i) the solver claims optimality upon termination, (ii) the final lower and upper bounds satisfy our optimality tolerances, and (iii) $\Delta_{p,s} < 10^{-3}$. As we detail in the following, to perform fair comparisons, we include additional safeguards to detect cases for which solvers make incorrect optimality claims.

To evaluate and compare the performance of different solvers on our test set, we make use of performance profiles, as described in [16]. The performance profile of a solver is a (cumulative) distribution function for a performance metric. Throughout this section, we use the ratio of the time that an algorithm takes to *solve* a problem versus the best time of all algorithms as the performance metric. For the purpose of constructing performance profiles, by *solve* we imply that the algorithm finds the best solution among all solvers for a given problem within the time limit. We utilize the `GAMS` performance tools [23] to construct all performance profiles. To account for trivial problems as we described in the previous section, we set `resmin`$=0.5$. As defined by the `GAMS` performance tools manual, `resmin` is the minimum resource time threshold. That is, if a solver reports a resource time below `resmin`, then it is increased to `resmin` before being used in ratios.

Table 1 Size statistics for the test set

	m	n	nz	nnz
(a) 980 NLPs from `PrincetonLib`				
Minimum	0	1	2	0
First quartile	0	3	7	4
Median	3	10	41	14
Third quartile	112	492	2347	691
Maximum	14,001	20,201	7,970,301	120,001
(b) 369 NLPs from `GlobalLib`				
Minimum	0	1	2	0
First quartile	4	5	20	6
Median	10	14	62	20
Third quartile	76	126	665	442
Maximum	26,758	19,314	128,411	31,261
	m	n	n_d	nz	nnz
(c) 250 MINLPs from `MINLPLib`					
Minimum	0	2	1	3	1
First quartile	10	11	6	52	10
Median	63	91	30	338	21
Third quartile	269	195	72	1441	127
Maximum	24,971	23,826	10,920	106,857	61,108
(d) 142 MINLPs from `IBMLib`					
Minimum	12	15	4	39	2
First quartile	212	131	40	653	14
Median	528	319	82	1355	36
Third quartile	1453	721	208	3582	80
Maximum	4981	2721	576	11,685	336

For each collection, we list the numbers of constraints (m), variables (n), discrete variables (n_d) (for MINLPs), nonzero elements in the constraints and objective (nz), and nonlinear elements in the constraints and objective (nnz)

4.1 Impact of proposed relaxation techniques on the performance of `BARON`

The cut generation and range reduction schemes of Sect. 2 and the hybrid LP/NLP-based lower bounding framework of Sect. 3, are implemented in `BARON 16.5.16`. To demonstrate the impact of these techniques, we will compare `BARON 16` against the same version of `BARON` but with all these techniques disabled. We will refer to the latter version of the solver as `BARON X`. `BARON X` will be restricted to utilize `MINOS 5.5` for local search, whereas `BARON 16` performs dynamic local search using `CONOPT 3.17A` [18], `IPOPT 3.12.3` [49], `MINOS 5.5` [37], `SNOPT 7.2-12.1` [26], and `FILTERSD 2` [15] as local NLP sub-solvers. Both

Table 2 Effect of proposed relaxation techniques on the performance of BARON for 756 NLPs and MINLPs from PrincetonLib, GlobalLib, MINLPLib, and IBMLib

	PrincetonLib	GlobalLib	MINLPLib	IBMLib	Total models
BARON 16 infinitely faster	200 (51%)	26 (23%)	12 (10%)	0 (0%)	238 (32%)
BARON 16 much faster	70 (18%)	11 (10%)	41 (34%)	93 (73%)	215 (28%)
BARON 16 faster	18 (4%)	8 (7%)	20 (17%)	17 (13%)	63 (8%)
Solvers perform the same	70 (18%)	57 (50%)	33 (27%)	9 (7%)	169 (22%)
BARON X faster	16 (4%)	7 (6%)	5 (4%)	6 (5%)	34 (5%)
BARON X much faster	19 (5%)	4 (4%)	10 (8%)	3 (2%)	36 (5%)
BARON X infinitely faster	2 (0%)	0 (0%)	0 (0%)	0 (0%)	2 (0%)

BARON 16 and BARON X use CPLEX 12.6.3 [30] as the default solver for LPs and MIPs.

To compare the performance of BARON 16 and BARON X, we first eliminate from the test set all problems that are trivial and problems for which both algorithms fail to return a feasible solution or cannot guarantee global optimality due to numerical difficulties. Subsequently, for a given problem, we classify the relative performance of the two algorithms with respect to their computational time, as follows:

(i) Solver A is considered infinitely faster than Solver B if Solver A solves the problem to global optimality within the time limit, while Solver B fails due to numerical difficulties or does not return a feasible solution upon termination.
(ii) A solver is considered much faster than another if it is more than 50% faster.
(iv) A solver is considered faster than another if it is faster by less than 50% but more than 10%.
(v) Solution times are considered the same, if they are within 10% of each other.

Comparative statistics for the test set are listed in Table 2. The first line of Table 2 provides the number and, in parentheses, the percentage of problems for which BARON 16 is infinitely faster than BARON X for each test library. The subsequent lines of the table provide similar statistics based on the classification described above. Overall, for 60% of the problems, the proposed relaxation techniques lead to significant performance improvements. In particular, for about one third of the problems, BARON X fails, whereas BARON 16 returns a globally optimal solution within the time limit. For another one third of the problems, the proposed techniques reduce the CPU time of the global solver by at least a factor of two. We observe performance degradations for about 10% of the test problems, most of which are due to incorporating more conservative cut generation and bounding strategies, as described in Sect. 2.5. In Table 3, we compare the number of problems solved to global optimality with and without the proposed relaxation techniques. As can be seen, the new relaxations increase the number of solvable models by 43% for PrincetonLib, 15% for GlobalLib, and 13% for both MINLPLib and IBMLib.

Next, we investigate the impact of the proposed techniques on *hard* problems, i.e., models that are not solvable by either of the two algorithms within the time limit, while a feasible solution is returned by at least one of the algorithms upon termina-

Table 3 Number of problems solved to global optimality within 500 s, with and without the proposed relaxation techniques

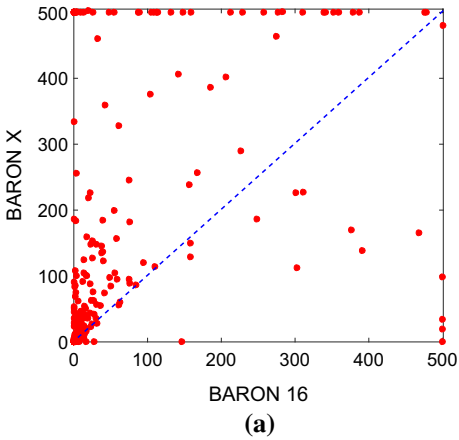
Test library	BARON 16	BARON X
PrincetonLib	732	512
GlobalLib	235	205
MINLPLib	168	149
IBMLib	136	120
Total models	1271	986

Table 4 Relative performance of BARON 16 and BARON X for 328 NLPs and MINLPs that are not solvable to global optimality within 500 s

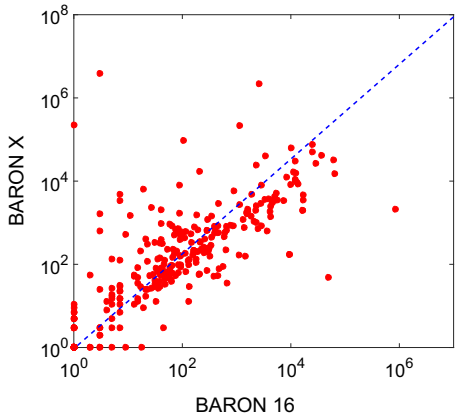
Test library	BARON 16 better	Same solutions	BARON X better
(a) Quality of best feasible solution			
PrincetonLib	149 (81%)	24 (13%)	11 (6%)
GlobalLib	49 (58%)	30 (35%)	6 (7%)
MINLPLib	23 (58%)	8 (20%)	9 (22%)
IBMLib	0 (0%)	5 (100%)	0 (0%)
Total models	221 (70%)	67 (21%)	26 (9%)
Test library	BARON 16 better	Same lower bounds	BARON X better
(b) Quality of lower bounds upon termination			
PrincetonLib	150 (82%)	14 (7%)	20 (11%)
GlobalLib	54 (64%)	17 (20%)	14 (16%)
MINLPLib	25 (63%)	6 (15%)	9 (22%)
IBMLib	4 (80%)	0 (0%)	1 (20%)
Total models	233 (74%)	37 (12%)	44 (14%)

tion. In Table 4, we compare the quality of lower and upper bounds of BARON 16 and BARON X after 500 s for hard problems from the test set. A solver is considered to provide a better upper bound (resp. lower bound), if the relative objective value difference (resp. relative lower bound difference) is greater than $\delta = 10^{-3}$. For objective values (resp. lower bounds) below one, we use absolute differences. Table 4a gives the numbers, and in parentheses the percentage, of problems for which BARON 16 returns a better solution, the two algorithms return the same solution, and BARON X returns a better solution for each collection. Table 4b provides similar statistics with respect to the quality of final lower bounds. The results in this table demonstrate that the proposed convexification methodology has a positive impact on the quality of lower and upper bounds for hard problems from the four test libraries.

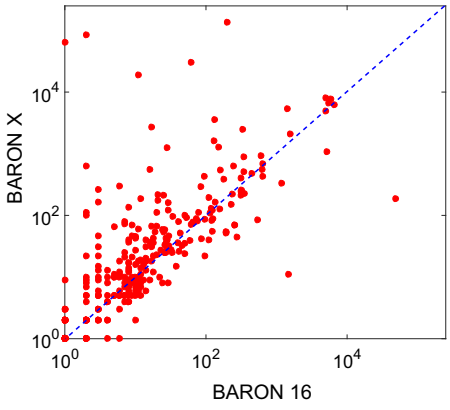
In Fig. 3, we compare the performance of BARON 16 and BARON X with respect to the following factors: (i) execution time, (ii) total number of nodes in the branch-and-bound tree, and (iii) maximum number of nodes stored in memory. Comparisons are performed on nontrivial problems for which neither of the two algorithms fails due to numerical difficulties and at least one of the algorithms finds the global solution



(a)



(b)



(c)

Fig. 3 Performance of BARON with and without the proposed convexification methodology for 375 problems from PrincetonLib, GlobalLib, MINLPlib, and IBMLib. In these figures, nontrivial problems that are solved to global optimality by at least one of the two algorithms are compared with respect to **a** CPU time, **b** total number of nodes in the branch-and-bound tree, and **c** maximum number of nodes stored in memory

Table 5 Relative computational cost of convexity exploitation operations in BARON

Test library	η_{cut} (%)	η_{conv} (%)
PrincetonLib	1.30 (3.82)	0.59 (5.52)
GlobalLib	0.81 (1.44)	0.02 (0.07)
MINLPLib	0.3 (0.7)	0.004 (0.03)
IBMLib	0.04 (0.1)	0.0 (0.0)

Table 6 BARON's performance for convex NLPs and MINLPs

Number of problems	PrincetonLib	GlobalLib	MINLPLib	IBMLib
Nontrivial models	708	336	232	142
Convex models	241	30	93	142
Solved by BARON X	108	17	78	120
Solved by BARON 16	220	30	85	136

within the time limit. Incorporating the proposed techniques in BARON results in average reductions of 38% in CPU time, 33% in total number of nodes in the branch-and-bound tree, and 26% in maximum number of nodes in memory.

In Table 5, we report the percentage of CPU time spent on generating cutting planes for convex intermediates as well as automatic convexity detection. By η_{cut}, we denote the average percentage of time spent on recognition and cut generation for the expressions described in Sect. 2, while η_{conv} denotes the average percentage of time spent on convexity detection. In addition, the numbers in parentheses denote the standard deviations from each mean value. As can be seen from this table, on average, less than one percent of the total time is spent on convexity detection, while the average time spent on generating cutting planes is slightly higher. For large convex problems with high-dimensional dense quadratic expressions, convexity detection may take up to 5 s. However, without convexity detection, BARON is not able to solve such problems within hours. Therefore, a careful time allocation for convexity detection based on the size and structure of the problem is of crucial importance.

Next, we examine the impact of the hybrid lower-bounding scheme of Sect. 3 on the performance of BARON for convex problems. In particular, we consider those problems whose continuous relaxations are proved to be convex in the first call to the convexity detector; that is, during preprocessing. In the first line of Table 6, we list the number of problems in each collection that are not solved to global optimality prior to the first call to the convexity detector. The second line contains the number of these problems that are found to be convex during preprocessing. In subsequent lines, we report the number of convex models that are solved to global optimality by BARON X and BARON 16, respectively. Clearly, employing highly efficient local solvers along with an examiner facility to test the optimality of the reported solution is very effective for continuous problems present in PrincetonLib and GlobalLib. For convex MINLPs of MINLPLib and IBMLib, however, the impact of nonlinear relaxations is less significant. This is mainly due to the fact that for these problems, BARON applies

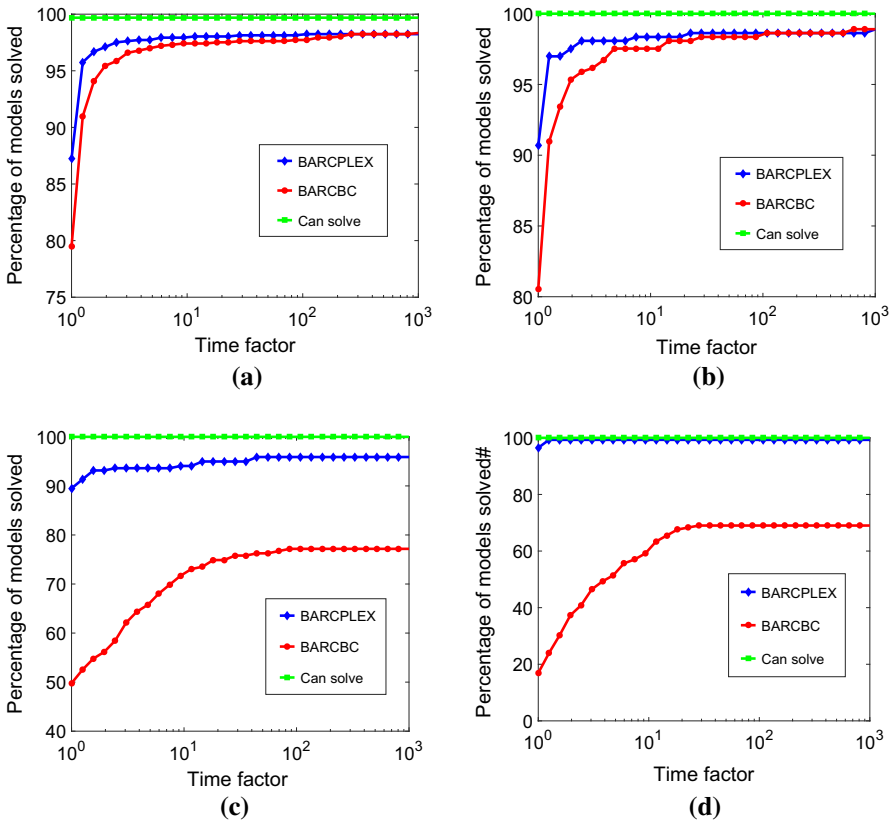


Fig. 4 Performance profiles of `BARON 16` using `CPLEX` as the LP/MIP solver (denoted by `BARCPLEX`) versus `BARON 16` using `CBC` as the LP/MIP solver (denoted by `BARCBC`) for problems from **a** `PrincetonLib`, **b** `GlobalLib`, **c** `MINLPLib`, and **d** `IBMLib`

MIP cutting plane and MIP relaxation technology, which are available in `BARON X` as well and often determine solution time requirements.

4.2 Impact of LP/NLP sub-solvers on the performance of `BARON`

Global solvers utilize LP/MIP and local NLP solvers at various stages during the global search. For instance, `BARON` uses LP codes for solving polyhedral relaxations of nonconvex problems as well as reducing the domain of variables via probing techniques (see [46] for details). Local NLP solvers are crucial for finding good feasible solutions, and they are used by `BARON 16` to construct hybrid LP/NLP relaxations. In this section, we examine the impact of various LP and local NLP solvers on the performance of `BARON`.

By default, `GAMS/BARON` uses the commercial code `CPLEX` [30] as the LP/MIP solver. Nonetheless, the Coin-OR LP/MIP solver `CBC` [14] is competitive with `CPLEX` on a wide range of problem types. Figure 4 shows the performance profiles of `BARON`

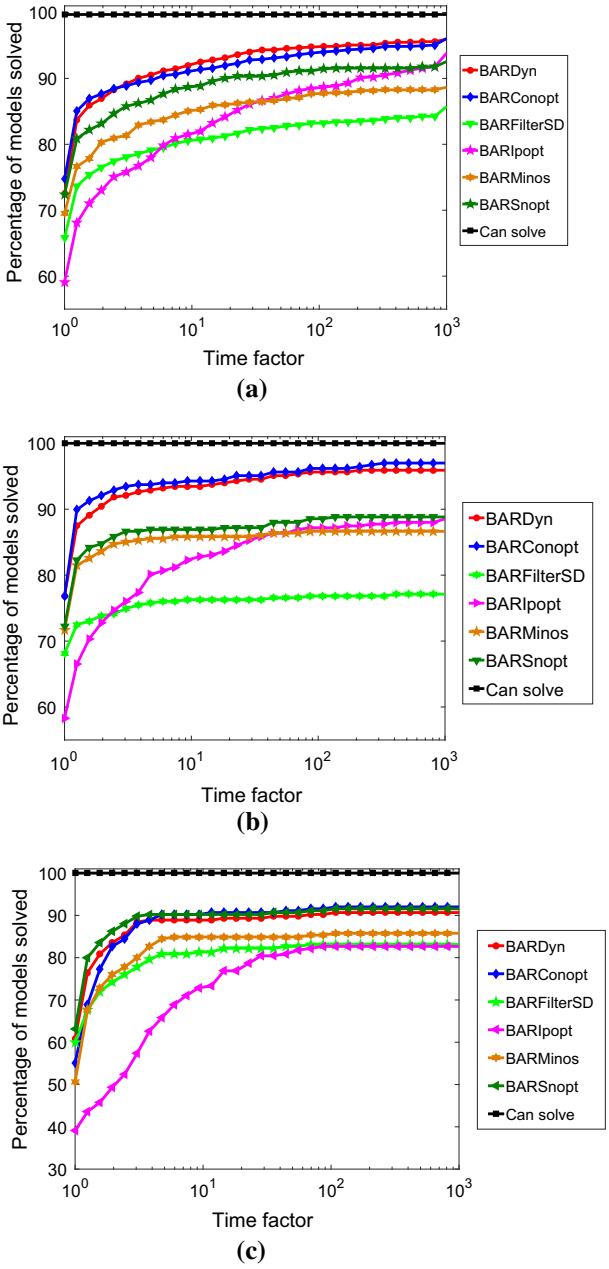
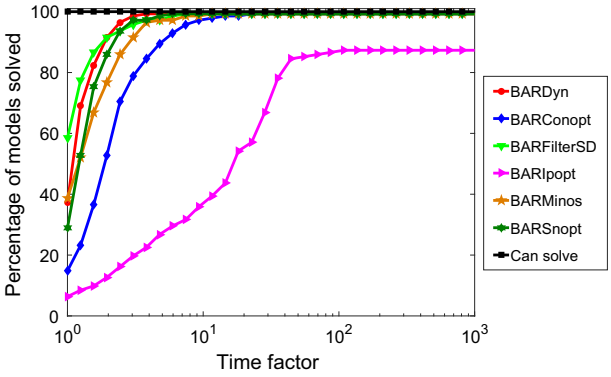


Fig. 5 Impact of various local NLP solvers on the performance of `BARON` for problems from **a** `PrincetonLib`, **b** `GlobalLib`, **c** `MINLPLib` and, **d** `IBMLib`



(d)

Fig. 5 continued

with CPLEX and CBC as its LP/MIP solvers. As can be seen from this figure, performance of the two algorithms is similar for continuous models while, for MINLP models, BARON with CPLEX outperforms BARON with CBC by a relatively large margin. This difference is due to the fact that CPLEX exploits special structures that are often encountered in combinatorial optimization problems and is therefore more effective in solving BARON's MIP relaxations.

Next, we examine the impact of various local solvers on the performance of BARON. To this end, we consider the following cases: (i) BARMINOS: BARON with MINOS 5.5 [37] as the local solver, (ii) BARSNOPT: BARON with SNOPT 7.2-12.1 [26] as the local solver, (iii) BARCONOPT: BARON with CONOPT 3.17A [18] as the local solver, (iv) BARIPOPT: BARON with CoinIPOPT 3.12.3 [49] as the local solver, (v) BARFilterSD: BARON with FilterSD 2 [15] at the local solver and, (vi) BARDyn: BARON with dynamic local solver selection strategy, which employs all aforementioned local solvers, as described in Sect. 3.2. Performance profiles for different local search strategies are shown in Fig. 5. While BARIPOPT is often slower than other solvers for all four collections, the choice of the best local solver varies depending on the problem type. For continuous models from PrincetonLib and GlobalLib, BARSNOPT and BARMINOS perform similarly, and they are outperformed by BARCONOPT. However, for MINLPs, BARSNOPT is the best solver and in particular for IBMLib, we observe a notable performance degradation for BARCONOPT in comparison to its performance on continuous problems. More importantly, it can be seen that BARDyn is competitive with the best static configurations for all test libraries. Comparing with the results of Sect. 4.1, we conclude that that the choice of LP/NLP solvers does not have a critical impact on the performance of BARON. For the most part, the superior performance of BARON 16 is due to the lower-bounding facilities proposed in this paper.

Finally, we discuss the failure rate of LP and local NLP solvers in the branch-and-bound tree. As we alluded to in Sect. 2.5, both LP and local NLP solvers occasionally make false optimality claims. Accepting incorrect solutions may lead to wrong results. Figure 6 shows LP/NLP subsolver failure rates in the branch-and-bound tree, on

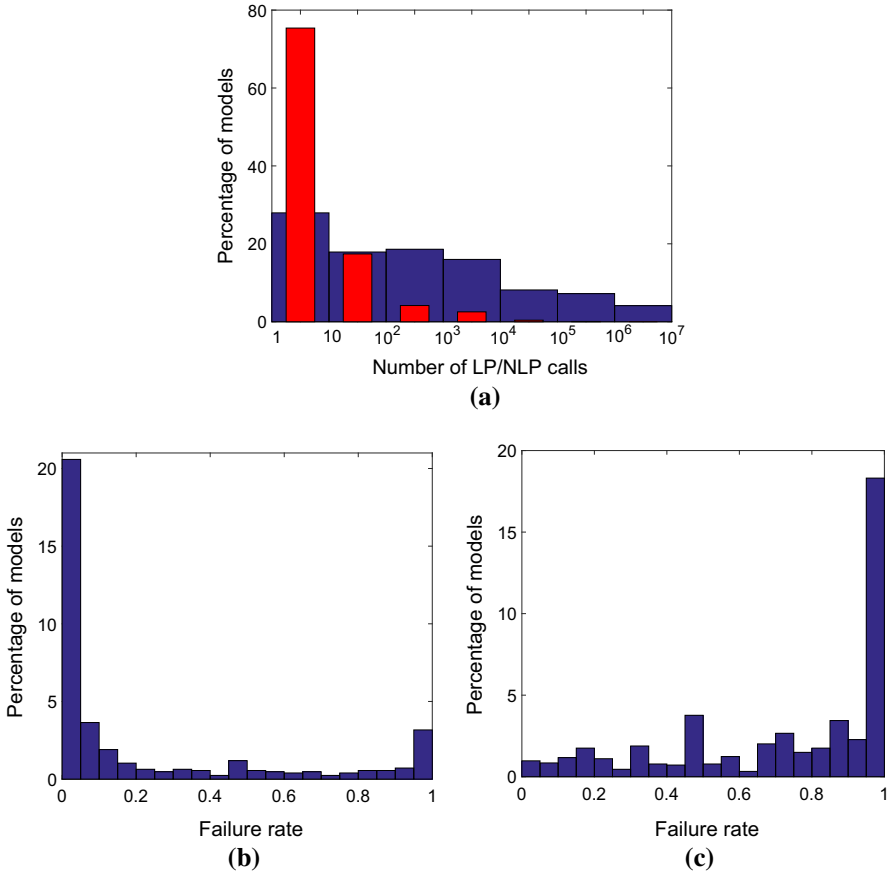


Fig. 6 Failure rate of LP and local NLP sub-solvers in BARON's search tree for 1740 NLPs and MINLPs from PrincetonLib, GlobalLib, MINLPLib, and IBMLib. In (**a**), blue bars represent the distribution of LP calls, while red bars represent the distribution of NLP calls. In (**b**, **c**), we have eliminated those models for which no sub-solver failure was diagnosed in the branch-and-bound tree by BARON's examiner. **a** Number of LP/NLPs calls in the branch-and-bound tree, **b** failure rate for CPLEX, **c** failure rate for local solvers (colour figure online)

a total number of 1740 NLPs and MINLPs from PrincetonLib, GlobalLib, MINLPLib, and IBMLib. All experiments are done with the default version of BARON 16, which utilizes CPLEX as the LP solver and dynamic local solver selection to optimize nonlinear sub-problems. By failure, we imply incorrect infeasibility and optimality claims for LP models, and incorrect local optimality claims for NLP sub-solvers. In particular, we say that a local solver fails if it declares the problem as locally optimal, while the reported solution does not pass the KKT test. At the time of this writing, BARON discards all infeasibility claims made by local NLP solvers. Verifying the infeasibility of convex NLPs requires the solution of certain auxiliary problems, and is the subject of future research. The distribution of the total number of LP/NLP calls over which the failure test is conducted is shown in Fig. 6a. In Fig. 6b, c, we have eliminated those models for which no failure has been reported. For 62% (resp.

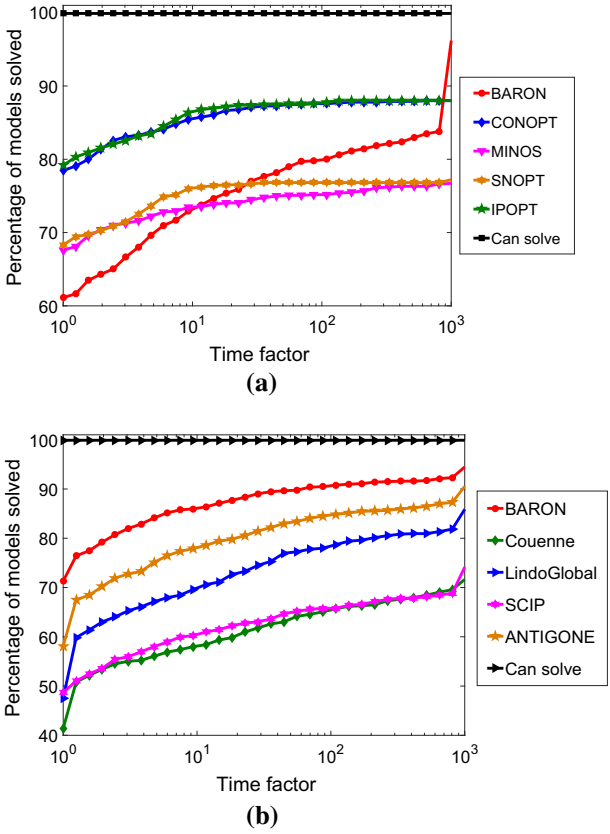


Fig. 7 Performance profiles of local solvers (**a**) and global solvers (**b**) for 980 NLPs from `PrincetonLib`

52%) of the models for which `CPLEX` (resp. local solver) is called at least once, the LP solver (resp. dynamic local search) does not make incorrect claims. For the remaining problems, the failure rate of `CPLEX` is mostly under 5%, while, for a few models, the LP solver makes incorrect optimality/infeasiblity claims for a high percentage of LP sub-problems. For local solvers, however, the failure rate is more evenly distributed, with the exception of a number of large-scale NLPs from `PRINCETONLib` for which none of the local solvers manages to return an optimal solution. This in turn highlights the importance of optimality verification steps. It is important to note that the failure rates of LP vs. NLP solvers should be interpreted carefully as, on overage, the number of LP calls is significantly larger than the number of NLP calls in `BARON`'s search tree (see Fig. 6a).

4.3 Comparisons with other local and global solvers

In this section, we provide extensive comparisons with several state-of-the-art local and global algorithms. We consider the following solvers:

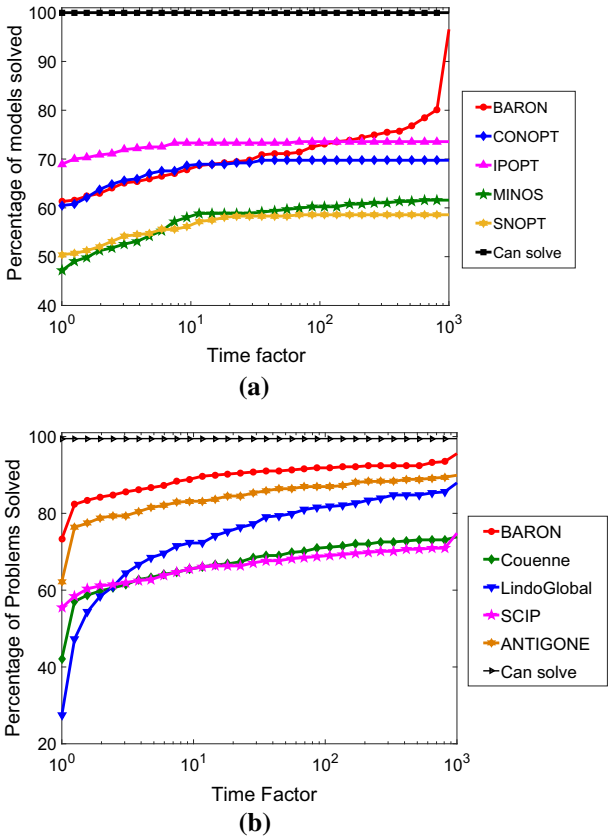


Fig. 8 Performance profiles of local solvers (**a**) and global solvers (**b**) for 369 NLPs from `GlobalLib`

(i) Local NLP solvers: `CONOPT 3.17A`, `IPOPT 3.12`, `MINOS 5.6`, `SNOPT 7.2-12.1`.
(ii) Local MINLP solvers: `AlphaECP 2.10.06` [50], `DICOPT` [19], `SBB` [25] all using `CPLEX` as the LP solver and `CONOPT` as the NLP solver and `BONMIN` [9] using IPOPT as the local NLP solver.
(iii) Global solvers: `Couenne 0.5` with `CBC` as the LP solver and `IPOPT` as the NLP solver, `Lindo API v 9.0` with `CONOPT 3.17A` as the NLP solver, `SCIP 3.2` with `CPLEX 12.6.3` as the LP solver and `IPOPT 3.12` as the NLP solver, `ANTIGONE 1.1` with `CPLEX` 12.6.3 as the LP solver and `CONOPT 3.17A` as the NLP solver.

We should remark that `GAMS/IPOPT`, which we use for the following comparisons, benefits from second-order derivatives and commercial factorization codes, neither of which are available in the version of `CoinIPOPT` that is incorporated by `BARON` as a local solver.

To conduct a fair comparison, for all subsequent comparisons, optimal solutions returned by all solvers are further tested using `GAMS/EXAMINER` [24]. The optimality

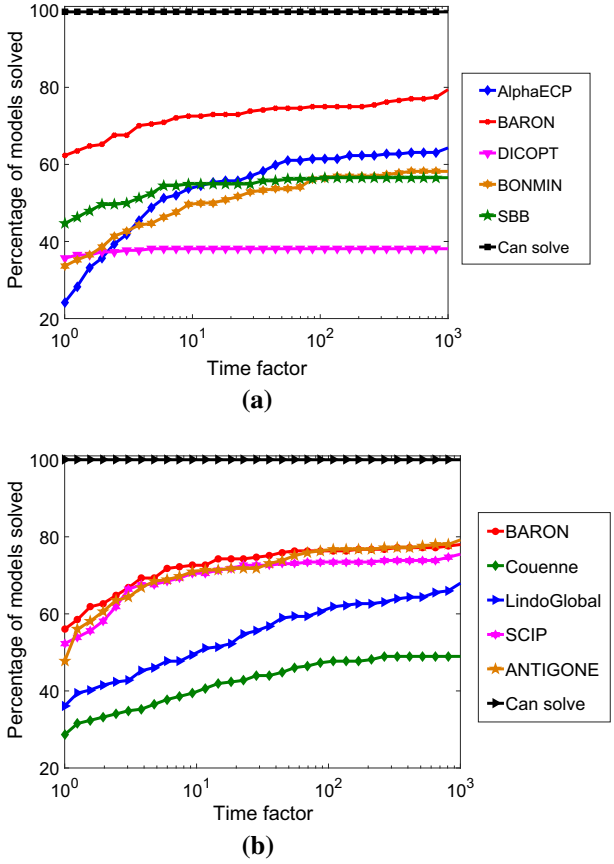


Fig. 9 Performance profiles of local solvers (**a**) and global solvers (**b**) for 250 MINLPs from `MINlPLib`

checks done in `EXAMINER` are first-order optimality conditions. `EXAMINER` takes the solution reported by the solver and tests for primal feasibility, dual feasibility, and complementarity slackness. While such a test is not sufficient to verify optimality for nonconvex problems, `EXAMINER` is an effective tool to identify many incorrect optimality claims made by different solvers. Since some of the global solvers utilized do not return dual values upon termination, we employ `EXAMINER`'s primal feasibility check for all our tests. We set `EXAMINER`'s feasibility tolerance to 10^{-5}, which is larger than the default value for the feasibility tolerance of the solvers under consideration.

Performance profiles of local and global solvers for the 980 NLPs from `PrincetonLib`, and the 369 NLPs from `GlobalLib` are shown in Figs. 7 and 8, respectively. In comparison to other global solvers, `BARON` is dominant for both test libraries, followed by `ANTIGONE` by about a 10% margin for all performance ratios. In comparison to local solvers, `BARON` is outperformed by `CONOPT` and `IPOPT` for `PrincetonLib`, as this collection includes many large-scale problems for which `BARON` is not efficient at this point. For the `GlobalLib` collection, `BARON` outperforms `CONOPT`, but requires about two orders of magnitude more CPU time to

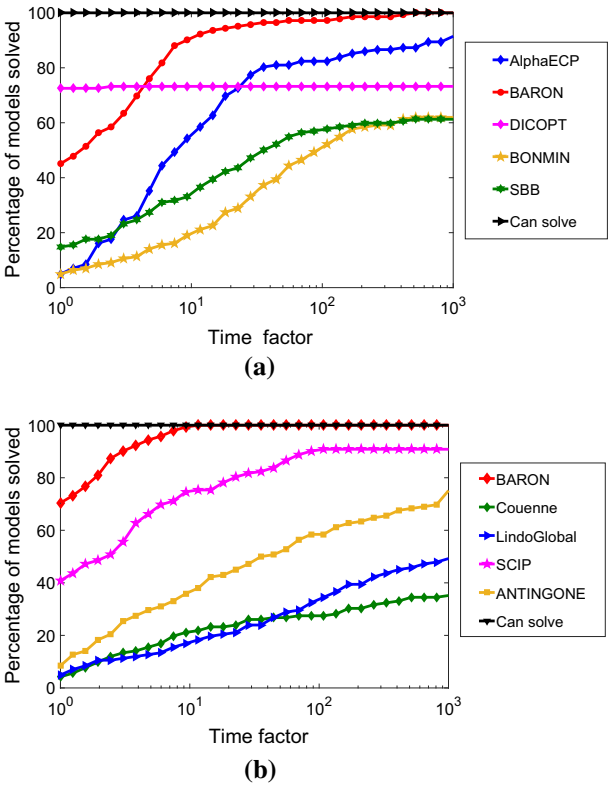


Fig. 10 Performance profiles of local solvers (**a**) and global solvers (**b**) for 142 MINLPs from IBMLib

solve more problems than IPOPT. It is interesting to note that, for both collections, BARON performs better than MINOS and SNOPT, both of which are highly efficient local solvers. This success is in part due to inability of local solvers to find global solutions of nonconvex problems and, more importantly, demonstrates the remarkable progress of global optimization algorithms and solvers over the past decade; BARON is capable of combining local solvers, such as MINOS and SNOPT, in ways that result in performance superior to that of each local solver in isolation. The jump at the end of the performance profiles of global solvers is merely due to problems that time out. Such problems are accounted for at the last tick in these graphs. Local solvers are not likely to time out and, as a result, their profiles are not likely to exhibit these jumps.

Performance profiles of local MINLP solvers and global solvers for the 250 MINLPs from MINLPLib are depicted in Fig. 9. For this test set, among global solvers BARON, SCIP and, ANTIGONE are quite competitive and are ahead of the other two global solvers Couenne and LINDOGlobal by a large margin. In comparison to local MINLP solvers, as can be seen in Fig. 9a, BARON is strongly dominant for this collection.

Finally, performance profiles for local MINLP solvers and global solvers for the 142 MINLPs from IBMLib are shown in Fig. 10. The continuous relaxation of all

problems in this library are convex. For this test library, BARON is ahead of both local MINLP and global solvers. BARON's superior performance for these problems is a result of its convexity detection tool together with cutting planes for perspective functions as well as various types of MIP cuts.

5 Conclusions

This paper demonstrates that convexity detection and exploitation is a powerful tool in global optimization of NLPs and MINLPs. We extended a widely-used polyhedral relaxation framework, by including cut generators for a variety of convex functions that appear frequently in applications. To capitalize on state-of-the-art in nonlinear programming algorithms, we developed a highly efficient convexity detector and proposed a hybrid LP/NLP-based lower bounding scheme that alternates between polyhedral and nonlinear relaxations at every node in the branch-and-bound tree. Results show that the proposed techniques significantly accelerate the branch-and-bound solver BARON and enable it to solve many more problems to global optimality.

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