Global optimization of mixed-integer models with quadratic and signomial functions: A review

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Global Optimization of Mixed-Integer Models with Quadratic and Signomial Functions: A Review

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Abstract

Mixed-integer quadratically-constrained quadratic programs (MIQCQP) and mixed-integer signomial optimization problems (MISO) are two important classes of mixed-integer nonconvex programs (nonconvex MINLP). This review discusses the practical applications of MIQCQP and MISO and covers algorithms designed to globally optimize them. We also describe numerical optimization software designed to solve these classes of problems.

Keywords: mixed-integer quadratically-constrained quadratic programs, mixed-integer signomial optimization problems, global optimization

AMS Classification: 90C26, 90C20, 90C57, 65K05

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1 Introduction

We begin in Section 2 by discussing the important application domains of mixed-integer quadratically-constrained quadratic programs (MIQCQP) and mixed-integer signomial optimization problems (MISO). Section 3 mathematically defines MIQCQP and MISO. Section 4 describes algorithmic components for globally optimizing MIQCQP and MISO including: Lagrangian-based global optimization (§4.1), automatic reformulations (§4.2), tight convex underestimators (§4.3), branching strategies (§4.4), bounds tightening (§4.5), and finding feasible solutions (§4.6).

This review will not cover this most general global optimization class of mixed-integer nonconvex programs (nonconvex MINLP); we refer the reader to the reviews of Floudas and co-workers [78, 91] for background on the state-of-the-art in global optimization, to the books edited by Floudas and Pardalos [80, 81, 82, 83, 84, 85] for a large quantity of research results, and to an array of excellent texts [73, 74, 205, 170, 198, 210].

There are reviews covering subclasses of MIQCQP and MISO. Anstreicher [23] discusses quadratic assignment problems and Misener and Floudas [158] cover pooling problems, a subclass of process networks problems with quality blending. See also the recent MIQCQP review of Burer and Saxena [45]. We refer the reader to the recent review of Bussieck and Vigerske [47] for detailed descriptions of generic MINLP solver software and limit the focus in Section 5 to numerical solver software deterministically addressing MIQCQP and MISO to global optimality.

Table 1: MIQCQP Test Suite of 665 Bounded Problems

Problem Class		# Cases	Discrete	# Nln Terms†	Source
	Pooling	19	✓	2 – 1350	[164]
Process	Water Systems	8	✓	46 – 260	[11, 12, 113, 186]
Networks	Crude Oil Scheduling	31	✓	54 – 3040	[125, 127, 128, 165, 166]
	Natural Gas Production	3	✓	34 – 2754	[130, 131, 196]
Computational	Point	14		6 – 630	[20]
Geometry	Circles & Polygons	36		23 – 931	[112]
Quadratic	BoxQP	90		205 – 3727	[46, 215, 216]
Programming	Standard QP	14		464 – 500500	[195]
	GLOBALLib	173		2 – 31210	[90, 153]
Test	MINLPLib	83	✓	4 – 31074	[48, 90]
Libraries	Other PerformanceLib	132		1 – 6984	
	Convex MIQCQP	20	✓	8 – 120	[42, 192]
Reformulated	Reform. GLOBALLib	32		2 – 34	[90, 153, 193]
Libraries	Reform. MINLPLib	10	✓	3 – 66	[48, 90]

† Range in the number of quadratic and bilinear terms for each problem class

2 Applications of Mixed-Integer Programs with Quadratic and Signomial Functions

2.1 MIQCQP Applications

Major applications of mixed-integer quadratically-constrained quadratic programs (MIQCQP) include quality blending in process networks, separating objects in computational geometry, and portfolio optimization in finance. Specific instantiations of MIQCQP in process networks optimization problems include: pooling problems [6, 17, 26, 36, 75, 98, 103, 104, 126, 157, 158, 159, 163, 164, 174, 220, 226], distillation sequences [9, 76, 86], wastewater treatment and total water systems [12, 18, 28, 37, 71, 94, 109, 113, 178, 181], hybrid energy systems [29, 30, 69], heat exchanger networks [59, 79], reactor-separator-recycle systems [119, 120], separation systems [191], data reconciliation [187], batch processes [136], crude oil scheduling [125, 127, 128, 129, 167, 166], and natural gas production [130, 131]. Computational geometry problems formulated as MIQCQP include: point packing [20, 60], cutting convex shapes from rectangles [112, 182], maximizing the area of a convex polygon [25, 27], and chip layout and compaction [67]. Portfolio optimization in financial engineering can also be formulated as MIQCQP [151, 184]. Table 1 lists a variety of practically-relevant MIQCQP problems and their sources.

2.2 MISO Applications

Mixed-integer signomial optimization problems (MISO) were originally proposed when convex posynomial geometric programs could not model important engineering applications [40, 150, 173]. Interesting domains employing MISO include: synthesizing heat exchanger networks [77, 180]; planning in a petrochemical production network [110]; finding the global minimum energy configuration of microclusters [147, 148]; designing heat-integrated nonsharp distillation sequences [10]; synthesizing complex nonisothermal reactor networks [120]; optimizing product portfolio selection [111, 137]; and designing a thermochemical-based

Table 2: MISO Test Suite of 264 Problems

Problem Class		# Cases	Discrete	Source
minlp.org	Belgian Chocolate Problem	4	✓	[57, 58]
	Cascading Tanks	8	✓	[97]
	Cyclic Scheduling and Control	1	✓	[72]
	Distillation Sep. Sequences	2	✓	[49, 50, 51, 52]
	Heat Exchanger Networks	3	✓	[70, 229]
	Metabolic Networks	2	✓	[101, 102]
	Multi-Product Batch Plants	4	✓	[100, 118, 231]
	Periodic Scheduling	13	✓	[55, 56]
	Supply Chain Design	2	✓	[230, 232]
	Unit Commitment	2	✓	[169, 235]
	Water Distribution Network	8	✓	[43, 61]
	Water Treatment Network	6	✓	[11, 12, 113, 186]
Test Libraries	GLOBALLib	87		[90, 153]
	MINLPLib	91	✓	[48, 90]
	MacMOOPLib	8		
	AMPL Book Lib	8		[93]
	Bonmin Test Set	10	✓	[42, 192]
Literature Problems		5		[228]

process superstructure to convert biomass, coal, and natural gas to liquid transportation fuels [30]. Table 2 lists several application domains that have been addressed using MISO.

3 Problem Definition

Both MIQCQP (§3.1) and MISO (§3.2) are, most broadly, instantiations of MINLP:

$$\begin{aligned} \min \quad & f_0(x) \\ \text{s.t.} \quad & b_m^{\mathrm{LO}} \le f_m(x) \le b_m^{\mathrm{UP}} \quad \forall\, m \in \{1, \ldots, M\} \\ & x \in \mathbb{R}^C \times \{0, 1\}^B \times \mathbb{Z}^I \end{aligned} \tag{MINLP}$$

where $f_m(x) : x \mapsto \mathbb{R}$.

3.1 MIQCQP Definition

This review considers mixed-integer quadratically-constrained quadratic programs (MIQCQP) of the form:

$$\begin{aligned} \min \quad & x^T \cdot Q_0 \cdot x + a_0 \cdot x \\ \text{s.t.} \quad & b_m^L \le x^T \cdot Q_m \cdot x + a_m \cdot x \le b_m^U \quad \forall\, m \in \{1, \ldots, M\} \\ & x \in \mathbb{R}^C \times \{0, 1\}^B \times \mathbb{Z}^I \end{aligned} \tag{MIQCQP}$$

where C, B, I, and M represent the number of continuous variables, binary variables, integer variables, and constraints, respectively. We assume that it is possible to infer finite bounds $\left[x_i^L, x_i^U\right]$ on the variables participating in nonlinear terms. MIQCQP accepts general integer variables and products involving discrete variables (*i.e.*, products of continuous-continuous, continuous-binary, continuous-integer, binary-binary, binary-integer, and integer-integer). In practical applications, quadratic matrix Q_m equivalently reformulates into upper triangular form. We alternately denote quadratic products as:

$$x^T \cdot Q_m \cdot x = \sum_{i=0}^{C} \sum_{j=i}^{C} Q_{m,i,j} \cdot x_i \cdot x_j \quad \forall\, m \in \{0, \ldots, M\}$$

3.2 MISO Definition

We define MISO as:

$$\begin{aligned}
\min \quad & \sum_{s=1}^{S_0} c_{s_0} \cdot f_{s_0}(x) + x^T \cdot Q_0 \cdot x + a_0 \cdot x \\
\text{s.t.} \quad & b_m^{\text{LO}} \leq \sum_{s=1}^{S_m} c_{s_m} \cdot f_{s_m}(x) + x^T \cdot Q_m \cdot x + a_m \cdot x \leq b_m^{\text{UP}} \quad \forall\, m \in \{1, \ldots, M\} \\
& x \in \mathbb{R}^C \times \{0, 1\}^B \times \mathbb{Z}^I
\end{aligned} \tag{MISO}$$

where C, B, I, and M represent the number of continuous variables, binary variables, integer variables, and constraints, respectively. We assume that it is possible to infer finite bounds $\left[x_i^L, x_i^U\right]$ on the variables participating in nonlinear terms and the variable powers $p_{s_m,c}$ are assumed to be constant real numbers. The signomial terms $f_{S_m}(x)$ are defined:

$$f_{s_m}(x) = \prod_{c=1}^{C} x_c^{p_{s_m,c}} \tag{1}$$

and the variable powers $p_{s_m,c}$ are assumed to be constant real numbers. Simplifying the interval analysis, we further assume that each variable power $p_{s_m,c}$ is either integral or irrational (*i.e.*, we disallow negative x_i if x_i participates in term $x_i^{1/3}$ because we assume that $1/3$ approximates an irrational real). Finally, we explicitly admit absolute values $|x_i|$ into the formulation because addressing MISO implicitly encompasses absolute values:

$$|x_i| = \sqrt{x_i^2}. \tag{2}$$

4 Global Optimization Algorithms for MIQCQP and MISO

This section discusses optimization methodology and algorithmic techniques that have been applied to MIQCQP. Specifically, we cover: Lagrangian-based global optimization approaches (Section 4.1), tight convex underestimators for MIQCQP (Section 4.3), automatically reformulating MIQCQP (Section 4.2), MIQCQP branching strategies (Section 4.4), bounds tightening (Section 4.5), and finding good feasible solutions (Section 4.6).

4.1 Lagrangian-based Global Optimization Approaches

The Global Optimization Algorithm, GOP, was the first rigorous deterministic global optimization algorithm to solve QCQP [87, 88, 221, 222, 224, 225]. The theoretical developments of the GOP were preceded by the global optimal search approach GOS [89], which was also applied to pooling problems but could not offer theoretical guarantees for global optimality. Based on duality theory and Lagrangian relaxation, the algorithm alternates between solving a projection of the primal problem and a series of relaxed dual problems. When the upper bounding problem (the projection of the primal problem) converges to the lower bounding problem (the series of relaxed dual problems), global optimality is attained.

After Floudas and Visweswaran [87] proved that GOP would find the global optimum for a range of problem classes, Visweswaran and Floudas [221] solved the three pooling problem test cases of Haverly [104] and qualitatively showed that their algorithm took an average of 15 iterations to converge for a variety of starting points. Visweswaran and Floudas [222] addressed the more complex problems of Ben-Tal et al. [36][1] and showed that their improved GOP algorithm took less than a minute to solve all of the test cases. Later, Visweswaran and Floudas [224, 225] integrated GOP into a branch-and-bound framework that reduced algorithmic complexity though pruning and reduction steps at each node in the branch-and-bound

[1] Actually, Visweswaran and Floudas [222] used problems from a technical report released a couple years before the Ben-Tal et al. [36] paper was published, but the problems are the same.

tree. Visweswaran and Floudas [225] demonstrated the efficiency of their algorithms, which were released in a package called cGOP [223], using the Haverly [104] and Ben-Tal et al. [36] test cases.

Other than the GOP algorithm, Ben-Tal et al. [36], Adhya et al. [6], and Almutairi and Elhedhli [17] have proposed Lagrangian approaches. To determine a lower bound on the standard pooling problem, Ben-Tal et al. [36] generated a dual to the problem in terms of the Lagrangian and developed a branch-and-bound algorithm to which generates a converging sequence of lower bounds (solutions to the dual) and upper bounds (local primal solutions).

Like Ben-Tal et al. [36], Adhya et al. [6] solved a series of lower bounding Lagrangian duals to converge on the global optimum, but their technique yields a tighter sequence of lower bounds because the dual is solved by iterating between a procedure for generating Lagrange multipliers and a technique for generating better cuts using the Lagrangian sub-problems. Recently, Almutairi and Elhedhli [17] suggested a new Lagrangian relaxation for the pooling problem and demonstrated that their relaxation is often tighter than previously-developed Lagrangian relaxations.

4.2 Reformulating MIQCQP and MISO

Automatic reformulations, while common in MIP, are relatively rare in MIQCQP and MISO [47]. The MIQCQP solver GloMIQO represents a major effort to elucidate special structure via reformulations and integrates reformulation techniques that can be implemented generically and applied universally. A stand-alone reformulation engine with no associated solver is ROSE, the reformulation-optimization software engine [135].

Two recommended MIQCQP formulation strategies include disaggregating bilinear terms [134, 210, 213] and adding redundant linear constraints to the model formulation [12, 113, 188]. The GloMIQO reformulation uses the observation that disaggregating bilinear terms tightens the relaxation of MIQCQP and actively takes advantage of any redundant linear constraints added to the model. Other reformulations for MIQCQP have taken the form of reducing the number of nonconvex bilinear terms [26, 36, 134]. For example, Ben-Tal et al. [36] showed that the dual of MIQCQP is sometimes smaller than the primal, Audet et al. [26] eliminated bilinear terms in the pooling problem through mass balances at the intermediate nodes, and Liberti and Pantelides [134] generalized the contribution of Audet et al. [26] to automatically eliminate unnecessary bilinear terms in MIQCQP. The GloMIQO 2.0 implementation adds bilinear terms to the model formulation to create tight reformulation-linearization technique relaxations.

Authors who refer to reformulations for MISO typically mean building an expression tree as first described by Smith and Pantelides [203]. These reformulations do not change the problem sctructure but rather establish interconnections between nonlinear terms.

Two complementary strategies for working with an expression graph are: constructing an operator-based factorable programming tree [34, 152, 203, 219] and dividing nonconvex expressions into terms that are addressed individually [7, 8, 19, 149]. The advantage of the vertical, expression tree data structure is that graph transversal techniques are easily exploited to generate tight convex underestimators and infer variable bounds based on tree relationships [34]. The complementary horizontal, term-based data structures easily admit multivariable relaxations that are specifically designed for particular functional forms. Previous work has demonstrated that operator- and term-based strategies are mutually reinforcing [95].

4.3 Tight Convex Underestimators

Tight convex underestimators are important for MIQCQP and MISO in the context of branch-and-bound global optimization. We begin by discussing the termwise *convex hull* of special functional forms and continue on to a variety of convex underestimators that are applicable under a variety of circumstances.

4.3.1 Convex Envelopes

McCormick [152] and Al-Khayyal and Falk [16] developed an efficient relaxation technique bilinear term $x_i \cdot x_j$ which yields the *envelope*, or tightest possible convex relaxation, of the term. The envelope is polyhedral [183], and, given a domain of interest $[x_i^L, x_i^U] \times [x_j^L, x_j^U]$, its convex and concave portions are given by Eqs. (3) and (4).

$$\text{Convex Envelope:} \qquad \max\{x_j^L \cdot x_i + x_i^L \cdot x_j - x_i^L \cdot x_j^L\ , x_j^U \cdot x_i + x_i^U \cdot x_j - x_i^U \cdot x_j^U\} \tag{3}$$

$$\text{Concave Envelope:} \qquad \min\{x_j^U \cdot x_i + x_i^L \cdot x_j - x_i^L \cdot x_j^U\ , x_j^L \cdot x_i + x_i^U \cdot x_j - x_i^U \cdot x_j^L\} \tag{4}$$

A termwise relaxation scheme replaces every occurrence of $x_i \cdot x_j$ with a new variable $w_{i,j}^{xx}$ and constrains the new variable with the following linear constraints:

$$w_{i,j}^{xx} \geq x_j^L \cdot x_i + x_i^L \cdot x_j - x_i^L \cdot x_j^L \tag{5}$$

$$w_{i,j}^{xx} \geq x_j^U \cdot x_i + x_i^U \cdot x_j - x_i^U \cdot x_j^U \tag{6}$$

$$w_{i,j}^{xx} \leq x_j^U \cdot x_i + x_i^L \cdot x_j - x_i^L \cdot x_j^U \tag{7}$$

$$w_{i,j}^{xx} \leq x_j^L \cdot x_i + x_i^U \cdot x_j - x_i^U \cdot x_j^L \tag{8}$$

Androulakis et al. [19] showed that the maximum difference between variable $w_{i,j}^{xx}$ and the bilinear term $x_i \cdot x_j$ is equal to $d_{\max} = \frac{1}{4} \cdot (x_i^U - x_i^L) \cdot (x_j^U - x_j^L)$, that is, proportional to the area of the domain. Algorithms using convex envelopes are most effective in small domains; preprocessing methods like those of Lodwick [141] are therefore helpful in uncovering implicit bounds.

Foulds et al. [92] implemented the bilinear envelopes of McCormick [152] in a global optimization algorithm, used the branch-and-bound algorithm designed by Al-Khayyal and Falk [16] to address the test cases of Haverly [104] and some larger, novel test cases. A number of other studies have used termwise relaxation of bilinear terms in a branch-and-bound algorithm (*e.g.*, [181, 210, 113]).

Convex hulls have been developed for a variety of MISO functional forms including: fractional terms [149, 209, 210]; trilinear terms [154, 155]; quadrilinear terms [53]; odd degree monomials [133]; signomial terms [143, 145, 150]; low-dimensional edge-concave terms [156, 206, 207, 208]; submodular functions [214]; and interesting products [114, 115, 149].

4.3.2 Reformulation-Linearization Technique (RLT)

The reformulation-linearization technique (RLT), adds redundant constraints to an MINLP model so that, when the problem is relaxed, the resulting underestimation is tighter than it would have been without the additional constraints [198]. Some RLT techniques automatically generate cuts for MIQCQP and MISO [24, 198, 199, 201, 202]; other RLT strategies are designed through close analysis of optimization problem classes such as: quadratic assignment [4], pooling [181, 210], *de novo* protein design [117], integrated water systems [113], scheduling batch processes [108], point-packing [20], and process networks [187]. The trade-off between these complementary approaches is that generic methodologies are useful when the best redundant constraints are not known *a priori* while redundant constraints designed for specific applications exploit the special structure of particular problems without adding extraneous cuts.

For the pooling problem, Quesada and Grossmann [181] integrated the reformulation-linearization technique of Sherali and Alameddine [199] into a branch-and-bound optimization algorithm. Tawarmalani and Sahinidis [211] proved that the formulation of Quesada and Grossmann [181] is tighter than both the *p*- and *q*- formulations and, using the *pq*-formulation, obtained fast solution times on all of the standard pooling problem test cases. Meyer and Floudas [157] introduced a piecewise, augmented RLT and described their success in underestimating a large-scale generalized pooling problem. For generic MIQCQP, Androulakis et al. [19], Sherali and Tuncbilek [201], and Audet et al. [24] augmented a feasibility-based bounds tightening (FBBT) scheme with redundant RLT equations. Audet et al. [24] designed a branch-and-cut method for quadratic programs using four classes of RLT linearizations.

Liberti and Pantelides [134] proposed an extension to the RLT technique that adds specific bilinear terms to the model formulation. The MIQCQP solver GloMIQO considers a variant of this strategy that, in the special case of quadratic assignment problems, automatically reduces to the Adams and Sherali [5] and Adams and Johnson [4] RLT-1 formulation. The GloMIQO implementation identifies all variable/equation and equation/equation products that do not introduce new bilinear terms into the model formulation [161]. Depending on the product, GloMIQO may directly add the equation to the model formulation, dynamically introduce the equation as a cutting plane, or use the equation in a bounds-updating strategy.

4.3.3 Difference of Convex Functions

The classical αBB method determines univariate quadratic perturbations that convexify twice continuously differentiable functions via an interval Hessian matrix [7, 8, 13, 14, 15, 140, 149].

In the more narrow case of MIQCQP, a recurring idea is convexifying the matrix Q_m; $m \in \{0, \ldots, M\}$ using a difference of convex (D.C.) underestimators [41, 54, 107, 123, 176, 175, 177, 234]; we refer to these as αBB underestimators because they specialize the generic results of Floudas and co-workers to MIQCQP [7, 8, 19, 140]. Anstreicher [21] showed that, no matter the choice of α parameter, a D.C. relaxation of MIQCQP is dominated by a relaxation combining McCormick [152] envelopes and a semidefinite condition. Based on this result [21], we avoid extensive computation generating the α parameters (*e.g.*, we do not solve an LP as proposed by Zheng et al. [234]). But αBB convexifications are important for an MIQCQP cutting plane strategy; generating αBB cuts is less computationally demanding than, for example, deriving vertex polyhedral cuts.

4.3.4 Vertex Polyhedral Facets

Rather than adding relaxations of redundant nonlinear constraints to the MILP relaxation of MIQCQP or MISO, an alternative set of techniques adds cuts to strengthen the relaxation of specific equations through eigenvector projections [54, 171, 185, 194], polyhedral facets [22, 31, 44], or the KKT necessary optimality conditions [215, 216]. The use of polyhedral facets is motivated by the following observation: although Eqs. (5) – (8) represent the convex hull of a single bilinear term, the sum of these termwise hulls in the MILP relaxation of objective or constraint $m \in \{0, \ldots, M\}$ does not necessarily generate the convex hull of m itself. Therefore, there has been work towards uncovering the vertex polyhedral properties of a bilinear objective or constraint to generate a family of valid cuts that characterize the convex hull [22, 31, 44, 183].

Edge-concave functions admit a vertex polyhedral envelope and therefore have a convex hull consisting entirely of linear facets [156, 206, 207, 208]. These polyhedral facets can be alternatively determined by solving an LP [31, 197] or finding dominance relationships. The derivation of the convex hull for trilinear monomials by Meyer and Floudas [154, 155] uses identical triangulation principles.

4.3.5 Semidefinite Programming

Multiple relaxations for MIQCQP have been proposed based on a semidefiniteness condition (*e.g.*, [20, 32, 46, 62, 179, 193, 194, 200, 233]). The relaxations are variants on the constraint:

$$X - x \cdot x^T \succeq 0. \tag{9}$$

For MIQCQP with $C \times B \times I$ nonlinearly-participating variables, these relaxations typically require order $(C \times B \times I)^2$ nonlinear terms when, in many practical instantiations of MIQCQP, the quadratic and bilinear terms participating in MIQCQP sparsely populate the possible nonlinearities. Observe, for instance, in the large-scale ten-plant generalized pooling problem of Meyer and Floudas [157] that there are 130 nonlinearly participating variables but only 750 bilinear terms; fewer than 4.5% of the 1.69×10^4 possible nonlinear terms are in the model formulation.

Semidefinite relaxations are not typically applied to large-scale MIQCQP; even carefully-constructed semidefinite convexifications of Saxena et al. [194] and Qualizza et al. [179] were only applied to MIQCQP with 50 or fewer variables. To our knowledge, the only available system addressing large-scale MIQCQP with semidefinite-like relaxations is GloMIQO [160, 161]. GloMIQO considers cuts on an expression representing the collection of nonlinear terms in MIQCQP:

$$\sum_{(i,j)\in T_Q} x_i \cdot x_j \tag{10}$$

where set T_Q is the set of pairs for which nonlinear term $Q_{m,i,j}$ exists in an equation m. Expression (10) is used to develop cutting planes for MIQCQP.

Semidefinite relaxations are also used in polynomial optimization [106, 105, 172]. Semidefinite relaxations have been coupled with a decomposition method for more effective polynomial optimization [116].

4.3.6 Eigenvector Projections

Rather than adding relaxations of redundant nonlinear constraints to the MILP relaxation of MIQCQP, an alternative set of techniques adds cuts to strengthen the relaxation of specific equations through eigenvector projections [54, 171, 185, 194].

Eigenvector projections are a common relaxation strategy for nonconvex quadratic programming problems [54, 171, 185] that also have been used for underestimating MIQCQP [194]. The major difference between the seminal strategy of Rosen and Pardalos [185] and the more recent effort of Saxena et al. [194] is that Saxena et al. [194] do not transform the variables participating in connected, nonconvex quadratic terms into separable terms but rather augment the relaxation of each quadratic expression:

$$x^T \cdot Q_m \cdot x + a_m \cdot x + c_m \cdot y \leq b_m \quad \forall\, m \in \{1, \ldots, M\}$$

with a convex relaxation of the N eigenvalues $\lambda_{m,n}$ and corresponding eigenvectors $v_{m,n}$ of Q_m:

$$\sum_{n=1}^{N} \lambda_{m,n} \left(v_{m,n}^T x\right)^2 + a_m \cdot x + c_m \cdot y \leq b_m \quad \forall\, m \in \{1, \ldots, M\} \tag{11}$$

The Saxena et al. [194] treatment is suited for MIQCQP because nonlinearities may appear in multiple equations within MIQCQP and variable transformation is therefore undesirable.

4.3.7 Piecewise-affine Underestimators

The idea of piecewise-affine underestimators comes from the observation of Androulakis et al. [19] that a bilinear envelope is tightest for small domains [113, 157]. Partitioning the domain *a priori* and constructing a series sub–envelopes, constructs a relaxation tighter than the parent envelope in the same domain. Because only one of the envelopes is active for a given domain point, we represent the problem using an MILP rather than an LP. Meyer and Floudas [157] and Karuppiah and Grossmann [113] successfully used *ab initio* domain partitioning to underestimate large scale generalized pooling problems (*i, e.*, mixed integer bilinear programming problems).

Based on the successes of Meyer and Floudas [157] and Karuppiah and Grossmann [113], Wicaksono and Karimi [226] and Gounaris et al. [98] proposed a total of 20 alternatives for formulating piecewise-linear relaxations. Furthermore, Gounaris et al. [98] comprehensively investigated the application of *ab initio* piecewise convex envelopes to tight and efficient relaxations of the pooling problem and suggested ways to better formulate large-scale problems such as the ones addressed by Meyer and Floudas [157] and Karuppiah and Grossmann [113]. Other groups who have used piecewise-linear underestimators are Bergamini et al. [37], who expedited the convergence of their Outer Approximation for Global Optimization Algorithm using the piecewise envelopes; Saif et al. [191], who used piecewise underestimation of bilinear terms to globally optimize a reverse osmosis network; Pham et al. [174], who coupled the piecewise underestimators with a fast-solving algorithm to generate near-optimal solutions; Hasan and Karimi [103], who partitioned both variables appearing in each bilinear term; and Misener et al. [163], who used piecewise envelopes to address the extended pooling problem.

Each of the previously-mentioned partitioning schemes requires a number of binary variables that scales linearly with the number of disjunctive segments in the relaxation. Vielma and Nemhauser [217] and Vielma et al. [218] recently proposed modeling piecewise functions with a number of binary switches that scales logarithmically with the number of partitions. Misener et al. [160, 164] proposed piecewise underestimators for bilinear terms with a logarithmic number of binary variables.

Piecewise affine underestimators have also been used in a number of MISO contexts including: well scheduling on petroleum fields [121, 122], gas lifting [162], water distribution networks [43], and stochastic programs from integrated process design [132].

4.4 Branching Strategies

Interesting branching strategies suitable for MIQCQP and MISO include simple heuristic strategies for determining the variable with the greatest associated error [7, 8, 24], ellipsoidal branching [107], strong branching [2], violation transfer [210, 211], branching on triangles [139], and reliability branching [2, 34]. The most popularly used technique, which is integrated into Couenne [34], GloMIQO [160, 161], and SCIP [39, 38], is reliability branching, a technique that integrates strong branching with a pseudocost heuristic to predict the best branching variable [2, 34].

4.5 Bounds Tightening for MIQCQP

Practical implementations of MIQCQP and MISO solver software rely heavily on bounds tightening to reduce the feasible space. Feasibility-based bounds tightening (FBBT), which uses interval arithmetic to place bounds on expressions by recursively overestimating each of the participating functions and operators, is the simplest and most computationally inexpensive technique [7, 8, 19, 24, 34, 168, 201, 202, 227]. An alternative, optimization-based bounds tightening (OBBT) methodology for determining these interval estimates is to minimize and maximize the expression under the bound constraints and possibly additional linear and convex constraints from the problem. These subproblems provide tighter bounds than interval arithmetic [149, 210]. A decreased number of nodes in the branch-and-bound tree may justify the increased computational effort needed to find better estimates.

FBBT and OBBT represent extremes. FBBT is cheap but not especially effective; OBBT is computationally demanding but may significantly reduce the bounds. The most interesting bound tightening techniques offer tighter bounds than natural interval extensions but are less computationally demanding than OBBT. These include: RLT-based bounds tightening [19, 24, 201], reduced cost bounds tightening [189, 190], quadratic equation constraint satisfaction [65, 66, 99, 124, 219], aggressive bounds tightening [34], and tightening based on pairs of linear inequalities [33]. Belotti et al. [35] carefully analyzed the convergence of a variety of interval-based techniques.

4.6 Finding Feasible Solutions

Finally, any branch-and-bound global optimization algorithm needs subroutines for finding feasible solutions. A common strategy is to initialize a local NLP solver at the node relaxation solution [7, 8, 34]. A suggestion for better performance from local NLP solvers is to avoid equality constraints with nonlinearities [68].

5 Global Optimization Software

We refer the reader to the recent review of Bussieck and Vigerske [47] for detailed descriptions of generic MINLP solver software. This section focuses on solver software for deterministic global optimization of MIQCQP and MISO.

αBB [7, 8, 19, 74, 149]

The primary contribution of the αBB code base is the implementation of a method determining univariate quadratic perturbations that convexify twice-continuously differentiable functions. This quadratic perturbation technique is integrated into a branch-and-bound algorithm addressing MINLP to ε-global optimality. Although αBB addresses the broader class of MINLP, it has specialized routines to handle MIQCQP via the convex envelopes of bilinear terms [16, 152]. MISO is addressed via specialized underestimators for univariate concave, trilinear, and fractional terms.

BARON [31, 210, 211, 212]

Like αBB, the BARON code base addresses general MINLP to ε-global optimality but specializes its approach for MIQCQP and MISO. In addition to relaxing bilinear terms using the convex hull, the BARON preprocessing routines detect connected multivariable terms within quadratic equations [31]. These connected multivariable terms are used to generate multidimensional cuts at the root node of the BARON branch-and-bound tree. Specialized relaxations for MISO include those for fractional [209] and submodular [214] terms. The bound reduction strategies within BARON are also applicable to MIQCQP and MISO [189, 190].

Branch-and-cut for QCQP [24, 25, 26, 27]

Audet et al. [24] discuss their implementation of a branch-and-cut global optimization algorithm for QCQP which made contributions to generating cutting planes and bound-updating strategies.

Couenne [34, 142]

Like αBB and BARON, Couenne addresses generic MINLP to ε-global optimality with specialized treatment for MIQCQP and MISO. There are novel branching strategies and feasibility-based bounds tightening advances within Couenne [33, 34, 35].

GloptiPoly [106, 105]

GloptiPoly is a Matlab/SeDuMi [204] add-on solving the Generalized Problem of Moments (GPM). The code builds a series of semidefinite programming relaxations of the GPM to converge to the global optimum.

GloptLAB [63, 64, 65, 66]

GloptLAB is a Matlab-based framework for solving quadratic constraint satisfaction problems [63]. The GloptLAB bounding and scaling strategies are particularly interesting [64, 65, 66].

GloMIQO [160, 161]

GloMIQO is an MIQCQP solver that detects and exploits an array of special mathematical structure components within MIQCQP. It consists of a reformulation, special structure detection, and branch-and-bound global optimization phase. The reformulations may increase the number of nonlinear terms in the model but also tighten the relaxation. The special structure detection phase focuses on convexity and edge-concavity. GloMIQO uses a number of relaxations including convex envelopes, RLT equations, αBB cuts, edge-concave facets, and eigenvector projections. Cuts are based both on individual equations and the collection of bilinear terms in MIQCQP.

LindoGLOBAL [96, 138]

Like αBB, BARON, and Couenne, LindoGLOBAL addresses generic MINLP to global optimality with specific routines for quadratic components.

SCIP [1, 3, 39, 38]

SCIP was originally developed as an mixed-integer programming (MIP) solver, but was extended to MIQCQP [39, 38] and then to MINLP [219]. SCIP recognizes several special structure components within MIQCQP including convexity and second-order cone constraints [39, 38]. For MISO, it reformulates an expression tree, detects convexity, and underestimates a variety of special functional forms [219].

SGO [143, 145, 144]
The signomial global optimization algorithm convexifies signomial terms through power and exponential transformations and uses piecewise affine transformations to converge to the global optimum. An extension of the SGO algorithm encompasses the more general class of MINLP [146].

6 Conclusion

This review has discussed recent advances in global optimization of MIQCQP and MISO, with a primary focus on large-scale, industrially-relevant problems formulated as MIQCQP and MISO. The key components of global optimization algorithms are discussed. We end with a discussion of numerical global optimization solver software suitable for MIQCQP and MISO.

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