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OCA PAD AMENDMENT - PROJECT HEADER INFORMATION

11/30/94

Active

Project #: E-24-644 Cost share #: E-24-330 Rev #: 5
Center # : 10/24-6-R7329-0A0 Center shr #: 10/22-1-F7329-0A0 OCA file #:
Contract#: DDM-9114489 Mod #: 1 Work type : RES
Prime # : Document : GRANT
Contract entity: GTRC

Subprojects ? : N CFDA: 47.041
Main project #: PE #: N/A

Project unit: ISYE Unit code: 02.010.124
Project director(s):
AL-KHAYYAL F A ISYE (404)894-3037

Sponsor/division names: NATL SCIENCE FOUNDATION / GENERAL
Sponsor/division codes: 107 / 000

Award period: 910901 to 950228 (performance) 950531 (reports)

Sponsor amount	New this change	Total to date
Contract value	0.00	82,909.00
Funded	0.00	82,909.00
Cost sharing amount		4,145.00

Does subcontracting plan apply ? : N

Title: NONLINEAR PROGRAMMING WITH QUADRATIC CONSTRAINTS

PROJECT ADMINISTRATION DATA

OCA contact: Jacquelyn L. Bendall 894-4820

Sponsor technical contact Sponsor issuing office

THOM J. HODGSON MARIA VALERIO
(202)357-5167 (202)357-9626

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Administrative comments -

AMENDMENT NO. 2 EXTENDS PROJECT TERMINATION DATE THROUGH FEBRUARY 28, 1995.

2-254

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NOTICE OF PROJECT CLOSEOUT

Closeout Notice Date 08/07/95

Project No. E-24-644 _____ Center No. 10/24-6-R7329-0A0_

Project Director AL-KHAYYAL F A _____ School/Lab ISYE _____

Sponsor NATL SCIENCE FOUNDATION/GENERAL _____

Contract/Grant No. DDM-9114489 _____ Contract Entity GTRC

Prime Contract No. _____

Title NONLINEAR PROGRAMMING WITH QUADRATIC CONSTRAINTS _____

Effective Completion Date 950228 (Performance) 950531 (Reports)

Closeout Actions Required:	Y/N	Date Submitted
Final Invoice or Copy of Final Invoice	N	_____
Final Report of Inventions and/or Subcontracts	N	_____
Government Property Inventory & Related Certificate	N	_____
Classified Material Certificate	N	_____
Release and Assignment	N	_____
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Comments _____
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Continues Project No. _____

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Project File	Y
Other _____	N
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Annual Progress Report

Nonlinear Programming with Quadratic Constraints
NSF Grant No. DDM-9114489

Faiz A. Al-Khayyal, Principle Investigator
School of Industrial and Systems Engineering
Georgia Institute of Technology

Funding for this project comprises full year support for one graduate student (beginning October 1991) and summer support for the principle investigator (beginning July 1992). We report herein on the accomplishments and progress achieved during the first full year of the grant. An unexpected medical condition, which required major surgery in December 1991 to correct, precluded the principle investigator from any progress in the six month period from January to June 1992, during which no charges were made to the grant. The research for that period will be completed during the six month no cost extension from October 1993 to March 1994.

The graduate students that were supported between October 1991 and September 1992 are foreign national Yinhua Wang (October-December, 1991) and U.S. national Timothy Van Voorhis (July-September 1991), with the latter student continuing his Ph.D. dissertation research under the grant.

Overall progress in the research area can be summarized as follows. A limited literature search was undertaken that focused on applications and methods that deal with quadratically constrained nonlinear programs. An in-progress paper was completed that developed an algorithm for quadratically constrained quadratic programs. Special cases of quadratically constrained nonlinear programs were investigated for the purpose of establishing and characterizing conditions under which solutions are guaranteed to exist or to be unbounded. In particular, we extended a sufficient condition for unboundedness of a quadratically constrained feasible region to necessary and sufficient conditions. Finally, we explored various aspects of a new linearization-relaxation technique for polynomial programs for the purpose of specializing and improving the results and methods to the treatment of quadratic constraints. Some promising preliminary results were obtained.

An elaboration on the accomplishments summarized above is presented next, starting with the literature search. Nonlinear programs arise in practically every major engineering field. Electrical engineering accounted for thirty of the ninety-five total references, mostly in control theory but also including power transmission, hydropower generation, robotic manipulation, circuit design, and signal and wave propagation. All required the solution of some nonlinearly constrained (often quadratic) programs. Chemical engineering had seven references in chemical process control, entropy minimization and parameter estimation. Structural design problems arising in aeronautical, civil, and marine engineering (designing aircraft wings, trusses, and undersea cables) were treated in seven references. Including other applications from ground water remediation to sound radiation control, there were a total of fifty-five references on engineering applications. Applications in the management and economic sciences yielded thirteen references on job scheduling, cost allocation, portfolio selection, setting transit fares, impact of energy prices on supply and demand elasticities, and finding equilibrium prices.

In addition to applications, the literature search classified the successful solution techniques for strengths and weaknesses. Quadratic programs have been solved by sequential linear programming, piecewise linear approximation, various active set methods, and by interior point methods. For nonlinear programs, successive quadratic programming was the most popular with variations concentrating on computing step-sizes, specifying descent functions, and updating the Hessian matrix. Other procedures that are gaining favor for some problems include interior point methods, descent methods relying on quadratic approximations, iterative linear programming, Tabu search, and approaches that decompose the problem and solve a series of problems in a lower dimensional space. The literature search was conducted by Tim Van Voorhis and a report detailing our findings is in preparation and should be ready by early next year.

The completed paper was in-progress at the time the grant was awarded. It was co-authored with Christian Larsen of the University of Odense (Odense, Denmark) and is entitled "Solving a General Quadratic Optimization Problem." A summary of the results will appear in the *Proceedings of the 1993 NSF Design and Manufacturing Systems Conference*. The method is based on outer approximation (linearization) and branch and bound with linear

programming subproblems. When the feasible set is nonconvex, the infinite process can be terminated with an approximate (possibly infeasible) optimal solution. Error bounds are derived that can be used to ensure stopping within a prespecified feasibility tolerance.

Some of the special cases of quadratically constrained nonlinear programs that were investigated by graduate assistant Yinhua Wang were the optimization of linear and quadratic objective functions over feasible sets defined by a single quadratic constraint, under different assumptions on the defining matrices. For the problem

$$\begin{aligned} \min \quad & c^T x \\ \text{s.t.} \quad & x^T Q x \leq b \end{aligned}$$

where $c \neq 0$, $b > 0$ and Q is symmetric, we have the following. When Q is positive definite, the optimal direction $-Q^{-1}c$ to the unique solution $-\sqrt{b/c^T Q^{-1}c} Q^{-1}c$ can be determined in $O(n^2)$ time using Gaussian elimination. When Q is either negative semidefinite or negative definite, the problem is unbounded. When Q is either positive semidefinite or indefinite, there are two cases: if c is in the orthogonal complement X^\perp of the homogeneous region $X = \{x : x^T Q x \leq 0\}$ and when $c \notin X^\perp$. In the first case, let t_1, t_2, \dots, t_k be a basis for X^\perp , then the problem is equivalent to

$$\begin{aligned} \min \quad & \tilde{c}^T y \\ \text{s.t.} \quad & y^T \tilde{Q} y \leq b \end{aligned}$$

where $\tilde{c} = (t_1, \dots, t_k)^T c$ and $\tilde{Q} = (t_1, \dots, t_k)^T Q (t_1, \dots, t_k)$ with positive definite \tilde{Q} . Since the latter problem can be solved in $O(n)$ running time, the main difficulty rests in determining a basis for X^\perp . In the positive semidefinite case, however, $X = \{x : Qx = 0\}$ so that $X^\perp = \text{aff}\{q_1, q_2, \dots, q_n\}$ where q_i is the i th column of Q and $\text{aff}\{\cdot\}$ denotes the affine hull of a collection of vectors. In the second case, when $c \notin X^\perp$, the problem is unbounded.

For the problem

$$\begin{aligned} \min \quad & x^T Q_0 x \\ \text{s.t.} \quad & x^T Q_1 x \geq b \end{aligned}$$

where $b > 0$ and Q_0 is positive definite, we have the following. If Q_0 is positive semidefinite, then the problem has optimal value of zero. If Q_0 is

anything else (indefinite, negative definite or semidefinite), then the objective function is unbounded so that existence of a solution to the problem depends on Q_1 . In order for the problem to be feasible, Q_1 cannot be either negative definite or semidefinite. If Q_1 is either positive semidefinite or indefinite, let t_1, \dots, t_k be a basis for the orthogonal complement of $\{x : x^T Q_1 x \geq 0\}$. As before, we can reduce the problem to

$$\begin{aligned} \min \quad & y^T \tilde{Q}_0 y \\ \text{s.t.} \quad & y^T \tilde{Q}_1 y \geq b \end{aligned}$$

where $\tilde{Q}_0 = (t_1, \dots, t_k)^T Q_0 (t_1, \dots, t_k)$ and $\tilde{Q}_1 = (t_1, \dots, t_k)^T Q_1 (t_1, \dots, t_k)$ with both \tilde{Q}_0 and \tilde{Q}_1 positive definite. Thus we only need to consider the case when both Q_0 and Q_1 are positive definite. This is a nonconvex program which can be approached in the following fashion.

A solution of the problem

$$\begin{aligned} \min \quad & \lambda \\ \text{s.t.} \quad & Q_0 x = \lambda Q_1 x \\ & x \neq 0 \end{aligned}$$

will yield an optimal direction and hence an optimal solution to the desired problem. The latter problem is equivalent to solving the collection of $n + 1$ problems

$$\begin{aligned} \min \quad & \lambda \\ \text{s.t.} \quad & Q_0 x = \lambda Q_1 x \\ & e^T x \leq -1 \end{aligned}$$

and for each $i = 1, \dots, n$

$$\begin{aligned} \min \quad & \lambda \\ \text{s.t.} \quad & Q_0 x = \lambda Q_1 x \\ & x_i \geq 1. \end{aligned}$$

Suppose the optimal solutions are $(\bar{x}^i, \bar{\lambda}^i)$ for $i = 0, 1, \dots, n$. (For infeasible problems, set $\bar{x}^i = 0$ and $\bar{\lambda}^i = +\infty$.) Let $i_* = \arg \min_i \{\bar{\lambda}^i\}$, then \bar{x}^{i_*} is an optimal direction for the desired problem. We note that since $\bar{\lambda}^{i_*}$ is the minimum eigenvalue of positive definite matrix $Q_1^{-1/2} Q_0 Q_1^{-1/2}$ and \bar{x}^{i_*} is the corresponding eigenvector, the $n + 1$ problems above should never be

unbounded and at least one has an optimal solution. It remains an open question whether procedures for these problems exist that are more efficient than solving for $Q_0^{-1/2}$ and the eigenvalues of $Q_1^{-1/2}Q_0Q_1^{-1/2}$.

In an unpublished manuscript entitled "Unboundedness of a Convex Quadratic Function Subject to Concave and Convex Quadratic Constraints," Caron and Obuchowska prove that the convex region defined by the intersection of a collection of convex quadratic constraints (call it R^V) is unbounded if and only if R^V contains a half-line. The same result holds for the non-convex region defined by the intersection of a collection of reverse convex quadratic constraints (call it R^C). The feasible region of the problem under consideration is $R = R^V \cap R^C$ and for this region, the authors prove that R is unbounded if it contains a half-line. That is, they were only able to find a sufficient condition for unboundedness of R . Under an independent study project with graduate student Gong Panjing, we were able to prove that R is unbounded if and only if it contains either a half-line or an unbounded quadratic arc on the boundary of R .

In a series of papers, H.D. Sherali *et al.* proposed a linearization-relaxation technique for polynomial programming problems. The procedure was specialized to a number of applications and research is ongoing. One such application which has not yet been addressed by Sherali is quadratically constrained quadratic programs. Our interest in the procedure is two-fold. First because it extends some ideas originally proposed by the principle investigator some fifteen years ago, and second because we believe that we can add a unique perspective to the approach that should enhance the utility and versatility of the theory. To that end we focused our preliminary investigation on studying the tightness of the linearizations for quadratic constraints with an eye to develop tighter relaxations.

The linearization-relaxation method treats every quadratic term x^2 over a bounded region $\ell \leq x \leq u$ as follows. The term is linearized by replacing it with a new variable, say w , wherever it appears in the problem and augmenting the feasible set of the problem by the constraints

$$\begin{aligned} w &\geq 2ux - u^2 \\ w &\geq 2\ell x - \ell^2 \\ w &\leq (u + \ell)x - \ell u \end{aligned}$$

Notice that this defines a linear overestimate of x^2 and a convex piecewise

linear underestimate of x^2 over $\ell \leq x \leq u$. Thus, the graph of x^2 is captured in a triangular region on the interval $[\ell, u]$. We experimented with several simple ideas for tightening the triangular region and thereby improving the linearization when x^2 appears in a constraint. The criterion we chose was the best reduction in volume of the triangular region by partitioning the interval $[\ell, u]$. The most reduction was achieved by bisecting the interval and constructing two triangles within the original that share a vertex at $(\frac{1}{2}(\ell + u), \frac{1}{4}(\ell + u)^2)$. Each of the smaller triangles has area $\frac{1}{32} \left[\frac{u - \ell}{2} \right]^3$, with the original triangle having area $\frac{1}{32} [u - \ell]^3$. Thus the area is reduced by a factor of four when splitting the interval. Moreover, the maximum vertical height in the triangle represents the maximum error of approximating x^2 by w and this occurs at the midpoint of the interval. Of course, to realize this gain we must double the number of linear constraints that augment the problem from three to six.

More challenging are the cross product terms xy which are linearized by replacing them with, say, z . With the bounds $a \leq x \leq b$ and $c \leq y \leq d$, the feasible set is augmented by the constraints

$$\begin{aligned} z &\geq dx + by - bd \\ z &\geq cx + ay - ac \\ z &\leq cx + by - bc \\ z &\leq dx + ay - ad \end{aligned}$$

The convex region in R^3 that captures the graph of xy is the convex hull of the four points (a, c, ac) , (a, d, ad) , (b, c, bc) and (b, d, bd) . The volume of this region depends only on differences $(b - a)$ and $(d - c)$, and not in the magnitude of the bounds, as in the previous case for x^2 . The volume is $\frac{1}{6}[(b - a)(d - c)]^2$ and the maximum error in estimating xy by z occurs at the center of the rectangular domain $\frac{1}{2}(a + b, c + d)$.

To give us an ability to experiment with our ideas, graduate research assistant Timonthy Vanvoorhis wrote a Pascal program that applied the linearization-relaxation technique of Sherali to quadratically constrained quadratic programs. Research in this area is ongoing and concrete results will be reported at a later date.

Given the limited quality time that was available to the principle investigator to devote to the project, we believe that the progress made to date meets or exceeds the goals set in the proposal for this juncture, keeping in mind that research will continue for six months at the end of the grant period during the no cost extension. We have concentrated our efforts on the development of new algorithms for obtaining approximate global solutions for the problems under investigation. We have begun to explore the limitations of existing and new algorithms for solving real problems. We have addressed the question of existence of solutions and have characterized this property for some quadratically constrained problems, while techniques for checking these conditions are still in the development stage. We have not yet begun to look into extending to the nonconvex case a technique developed by the principle investigator based on the concept of shrinking and rotating boxes that contain the feasible set. Instead we concentrated on the linearization-relaxation technique which we believe to be more promising at this time.

Turning to a summary of the work to be performed during the succeeding budget period, we plan to wrap up and clean up the preliminary results reported earlier. Technical reports and conference presentations will be completed on the literature search and on the necessary and sufficient conditions for unbounded convex sets. We shall experiment further with improvements to the linearization-relaxation technique and test our ideas on sample problems using the code we developed. Any substantive findings will be disseminated in a computational study. We also plan to devote some effort into deriving good error bounds and heuristic approximation techniques for quadratically constrained quadratic programs. An important and interesting problem, which has not been looked at in the literature, is to find a feasible solution from a near feasible solution for these problems. The latter might be obtained from an outer approximation technique and the former would significantly contribute to tightening *a posteriori* error bounds. We have some preliminary results on this problem, and we anticipate the development of a convergent algorithm for special cases of this problem. Finally, we have some early results on transcending from linearizations to quadratic convexifications to obtain tighter yet still tractable approximations to nonconvex programs. Some of this research involves convex underestimating functions of more general quadratic forms than considered to date, but it is too early to predict the value of these ideas at this time.

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NATIONAL SCIENCE FOUNDATION FINAL PROJECT REPORT

PART I - PROJECT IDENTIFICATION INFORMATION

1. Program Official/Org.	Pius J. Egbelu - DMII	
2. Program Name	OPERATIONS RESEARCH & PRODUCTION SYSTEMS	
3. Award Dates (MM/YY)	From: 09/91	To: 02/94
4. Institution and Address	GA Tech Res Corp - GIT Administration Building Atlanta GA 30332	
5. Award Number	9114489	
6. Project Title	Nonlinear Programming with Quadratic Constraints.	

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PART IV -- FINAL PROJECT REPORT -- SUMMARY DATA ON PROJECT PERSONNEL

(To be submitted to cognizant Program Officer upon completion of project)

The data requested below are important for the development of a statistical profile on the personnel supported by Federal grants. The information on this part is solicited in response to Public Law 99-383 and 42 USC 1885C. All information provided will be treated as confidential and will be safeguarded in accordance with the provisions of the Privacy Act of 1974. You should submit a single copy of this part with each final project report. However, submission of the requested information is not mandatory and is not a precondition of future award(s). Check the "Decline to Provide Information" box below if you do not wish to provide the information.

Please enter the numbers of individuals supported under this grant.
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	Senior Staff		Post-Doctorals		Graduate Students		Under-Graduates		Other Participants ¹	
	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.
A. Total, U.S. Citizens					1					
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Asian										
Black, Not of Hispanic Origin										
Hispanic										
Pacific Islander										
White, Not of Hispanic Origin	1				1					
C. Total, Other Non-U.S. Citizens					1					
Specify Country										
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2.										
3.										
D. Total, All participants (A + B + C)	1				2					
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³ A person having a physical or mental impairment that substantially limits one or more major life activities; who has a record of such impairment; or who is regarded as having such impairment. (Disabled individuals also should be counted under the appropriate ethnic/racial group unless they are classified as "Other Non-U.S. Citizens.")

AMERICAN INDIAN OR ALASKAN NATIVE: A person having origins in any of the original peoples of North America and who maintains cultural identification through tribal affiliation or community recognition.

ASIAN: A person having origins in any of the original peoples of East Asia, Southeast Asia or the Indian subcontinent. This area includes, for example, China, India, Indonesia, Japan, Korea and Vietnam.

BLACK, NOT OF HISPANIC ORIGIN: A person having origins in any of the black racial groups of Africa.

HISPANIC: A person of Mexican, Puerto Rican, Cuban, Central or South American or other Spanish culture or origin, regardless of race.

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Final Report
Nonlinear Programming with Quadratic Constraints
NSF Grant No. DMII-91-14489

Faiz A. Al-Khayyal, Principle Investigator
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Georgia Institute of Technology
Atlanta, Georgia 30332-0205

28 July 1995

Abstract

This project is concerned with developing computationally efficient procedures for solving optimization applications involving quadratic constraints. Such constraints are usually linearized in practice which leads to less precise modeling of the application. Availability of robust methods for global optimization of quadratically constrained optimization problems would improve the solutions of existing problems because better models can be applied.

The proposed procedure is a branch-and-bound method which is based on rectangular partitions and piecewise-linear under and overestimations that prescribe linear programming subproblems. The overall procedure is guaranteed to converge to a global solution. We report on results of experiments on computational enhancements to accelerate convergence and allow for the solution of larger applications than currently possible. Preliminary results are promising and suggest that a significant improvement in the overall algorithm is an achievable goal.

Enhancements dealt with include: (i) improving the lower bound, obtained from solving linear programming subproblems, by using augmented Lagrangian functions to solve tractable duals of the subproblems; (ii) finding good feasible points early by using Newton and Interval-Newton methods, and by using problem-specific heuristic techniques; and (iii) improving the convexifications of the subproblems while keeping them computationally tractable. Preliminary results in all three areas are inconclusive. Ongoing research to fully develop the most promising ideas is underway and will be reported at a later date.

1 Introduction

One of the most widely studied problems in optimization is the quadratic program, in which a quadratic objective function is minimized over a set of linear constraints. While several useful algorithms have been developed to solve problems of this sort, this formulation is inadequate for many industrial and engineering applications. Nonlinear constraints arise naturally in engineering to represent natural or empirical laws that govern the behavior of the system being modeled. Analysis of highly nonlinear engineering systems frequently resorts to quadratic approximations that are valid within some acceptable parameter ranges. However, problems with higher-order polynomials functions can be rewritten as *equivalent* quadratically constrained problems. For example, each x^7 term can be replaced by y_3x with the added constraints $y_1 = x^2$, $y_2 = y_1^2$, and $y_3 = y_1y_2$. Here, three new variables and three quadratic equality constraints are needed to represent x^7 , so any procedure based on quadratic reformulation must appeal to large scale optimization algorithms for quadratically constrained nonlinear programs of the form:

$$\begin{array}{ll} \text{Min} & x^t Q_0 x + c_0^t x \\ \text{subject to} & x^t Q_i x + c_i^t x \leq d_i, \quad i = 1, \dots, m. \end{array}$$

While this program is encountered regularly in a wide variety of areas, it is often very difficult to solve. A brief survey of current Operations Research literature reveals that these programs remain largely unstudied. More recent developments in Semidefinite Programming have revived interest in the convex version of the above problem which can be treated as a tractable semidefinite program, but this approach holds little promise for the nonconvex version of the problem, which is the focus of this research effort. General global optimization algorithms can be used for this class of problems, but these procedures are neither broadly-applicable nor practical for the larger instances of the problem which would be encountered in real-world applications. The following examples are presented as applications for which improved solution techniques would have an immediate impact.

2 Applications

Since variances are expressed as quadratic functions, stochastic environments naturally tend to give rise to quadratically constrained programs with linear or quadratic objective functions. Avram and Wein [7] consider a product design problem from the semiconductor industry. In this problem, the chip sites on a semiconductor wafer are allocated to the various types of chips. The variability of the wafer fabrication process complicates the problem. Hence, one possible objective function minimizes the maximum variance of a random variable T_k which describes the number of sets of nondefective type-k chips per wafer. While citing the difficulties posed by this objective, which results in a quadratically constrained minimization problem, the authors provide results for small instances of this problem, where 4 types of chips yield 4 quadratic constraints.

Probabilistic systems are often described mathematically by the chance-constrained program. Denardo and Tang [12] model a Markovian production system, where jobs move between manufacturing activities randomly. The model makes use of a linear control and relies on chance constraints to ensure, with a very high probability, both that buffer stock stays nonnegative and that production flows stay within each sector's capacities. This program is shown to be log-convex

and each sector has only three constraints, thus making the problem solvable using standard codes. In a similar approach, Weintraub and Vera [32] mention the usefulness of chance constrained linear programs in areas such as energy planning, industrial production, capital budgeting, and water system planning. Their particular algorithm is demonstrated by solving a chance constrained problem in the area of forest planning, by considering the randomness in future timber growth. In this case, feasible solutions are not difficult to find, and hence a cutting-plane algorithm is used to solve instances with up to 34 chance constraints. Similar constraints are used by Pourbabai and Seidmann [26] in a design of a branching system in telecommunications. This system consists of several parallel nonidentical communication devices with finite input buffers. Their models seek to maximize overall system throughput, and employ chance constraints to ensure that the probability of congestion (i.e. that more messages are sent to a device than its input storage capacity allows) is sufficiently small. Suggested algorithms are given which rely greatly on the structure of the particular application. The algorithm used in the most difficult case relies on a dynamic programming approach to solve the program in pseudo-polynomial time.

Production and scheduling problems provide several opportunities for applications of quadratically constrained quadratic programs. Gallego and Moon [17] seek to determine a multiple product, single facility cyclic schedule to minimize holding and setup costs. In this case, the possibility of externalizing setup operations is considered. Setup operations are said to be externalized if the production process is interrupted for all setup operations. This reduces setup time and holding costs but increases setup costs. The resulting model contains one fractional term which divides the setup time variable s_i by the cycle length variable t_i . By creating a new variable r_i such that $r_i t_i = 1$, this problem could be formulated as a bilinear program. Since the given formulation includes only one nonlinear constraint, all other terms may be expressed as a function of the Lagrange multiplier associated with this constraint. A search technique is used to find the optimal value for this multiplier and then all other terms are easily calculated.

Scheduling bottleneck operations is studied by Hum and Sarin [21]. An especially difficult problem arises when an entire lot must be processed before any part of that lot may be consumed. Decision variables for this model include N_i which is the number of setups (or production runs) for product i per unit time and x_i which is the number of units of product i produced per unit time. The N_i variables require the existence of another decision variable m_i which must satisfy the equation $m_1 N_1 = m_2 N_2$. Although this program is further complicated by integer restrictions, relaxing these results in a bilinearly constrained program, where the m variables are multiplied with both x and N variables. For the given examples each m variable could take on a very limited number of values. Hence, it was not computationally difficult to enumerate every possible vector of m variables and solve corresponding linear programs for each of these possibilities.

Efficiently utilizing production resources is also studied by Ahmadi and Matsuo [2] as they consider the problem of allocating pick-and-place robots which put electrical components on circuit boards to the various families of items at each stage of the production process. The objective is to minimize the total time to complete all jobs. The model employs variables T_{ij} , which represent the time assigned to production of item j in family i , and x_{ik} , which is the number of machines allocated to family i at stage k . The program is then given as minimizing the maximum completion time of any family i , which is given by $\sum_j T_{ij}$. A bilinear constraint is introduced by requiring that $T_{ij} x_{ik} \geq p_{ijk}$, where parameter p_{ijk} is the total processing time for item j in family i at stage k . Again, this program features integrality requirements, but relaxing these restrictions yields a bilinearly constrained program. Due to the difficulty of this problem, the authors do not attempt

to solve their program to optimality. Rather, the Lagrangian function is used to dualize nonlinear constraints and find lower bounds. Heuristics are suggested to find upper bounds. Solutions obtained are of varying quality, with all being within 7.5 percent of optimality.

Operations Research also features a variety of location problems, some of which may be best formulated with quadratic constraints. Benchakroun, Ferland, and Cleroux [10] introduce a model to specify the distribution system for an electrical power industry. The objective function seeks to minimize the sum of all costs, including those associated with maintenance, investment in substations, feeders, and voltage regulators, and energy loss in the feeders. The resulting program has a nonlinear objective and bilinear constraints, which feature both integer and continuous variables. By adding variables, the objective could be restated in quadratic form. In this application, a Bender's decomposition method is used to solve subproblems and generate additional cuts. Considerable effort is devoted to transforming the problem into a form which can be solved more efficiently. Solutions are given for small instances with 2 substations and 15 load locations.

Network design is encountered in a different context by Gavish [18], who considers the design problem faced by managers of computer networks when they must set up a new backbone network or expand an existing one. This network design consists in simultaneously selecting the locations for placing network control processors, deciding on the set of links which connect backbone nodes, selecting links of end-users to the network, and selecting routes used by end-users at minimum cost. This program also is a nonlinear combinatorial optimization problem which could be formulated as a bilinear one by replacing variables which are currently in the denominator of some term. Once again, both lower and upper bounds are found, instead of an exact solution. A subgradient optimization procedure is used to solve the Lagrangian relaxation of the original problem to obtain a lower bound. Greedy and partial-enumeration heuristics are used to find an upper bound.

The popular facility location problem becomes a quadratically constrained one when it is extended to multiple periods by Balakrishnan, Jacobs, and Venkataramanan [8]. This extension studies the facility layout problem under the two assumptions of changing demand, which could result in various optimal (or even near-optimal) layouts for different time periods, and a limited amount of funds for rearranging the layout between periods. The objective seeks to minimize the sum of rearranging costs and material flow costs. Decision variables are x_{tij} , a 0-1 variable for locating department i at location j in period t , and y_{tijl} , a 0-1 variable for shifting department i from location j to l at time t . Hence, a quadratic constraint is introduced of the form $y_{tijl} = x_{(t-1)ij}x_{tij}$. Two approaches are tested, a dynamic programming algorithm and a constrained shortest path algorithm. Since the dynamic programming approach is purely enumerative and the constrained shortest path technique combines enumeration with the simplex method, the latter procedure works much better for larger instances. The largest example solved considered an instance with 20 departments and 4 periods.

Another version of the facility location problem is studied by Jeul and Love [22]. The minimax location problem occurs when decision-makers locate a new facility at the location which will minimize the maximum distance from the new facility to any member of a set of existing facilities. This objective is used in locating facilities such as fire stations, hospitals, or military detection devices, each of which must be as close as possible to all of its targeted customers. This problem is easily demonstrated to consist of minimizing a linear objective subject to quadratic constraints. While no test results are given, solving the dual problem is suggested.

Various programming formulations encountered within the area of game theory also may be solved as quadratically constrained quadratic programs. Kostreva, Ordoyne, and Wiecek [24] pro-

pose an algorithm for solving multiple-objective programming problems with polynomial objectives and polynomial constraints. The algorithm is demonstrated by solving a problem in two-person game theory. A locally efficient point is found by minimizing a linear objective and moving both polynomial objective functions into the problem as constraints. For a small instance (3 constraints, including 2 original objectives), the Lagrangian matrix is given and algebraic methods are used to find all efficient points.

The bilevel programming problem arises from game theory applications in a variety of contexts. Anandalingam and Friesz [6] survey this problem and describe the associated two-person game. In this game, the “leader” selects his decision vector first, then the “follower” selects his decision. Hence the leader’s problem is to maximize a linear program in x (his decision space) and y (the follower’s decision space), where y is the optimal solution to the linear program which will confront the follower after the x decisions are known. This model is especially appropriate when a policy-maker must make decisions which take into account the likely response of a group of constituents. There are a number of different approaches to this problem, one of which uses the Karush-Kuhn-Tucker optimality conditions to form a bilinear program whose solution will give the optimal decision vector for both x and y . Suh and Kim [31] introduce a few applications of this program, in which the public sector is the leader of the game, and the private sector is the follower. These areas include natural resource management, project selection, strategic planning for the agricultural sector, and regional development. In particular, they consider the transportation planning problem, for which the public sector constructs new transportation systems, improves capacities, and regulates services and prices. The private sector then chooses locations of production, modes of transportation, and shipment routes. To solve this application, a descent-type algorithm is introduced which relies on derivative information of the lower level problem to calculate the optimal solution to the upper level problem.

A more complex example of bilevel linear programming, taken from a real-world application, is presented by Ben-Ayed, Blair, Boyce, and LeBlanc [9], who construct a program for optimizing the investment in the inter-regional highway network of a developing country. Again, an iterative algorithm is developed which solves the lower problem separately. In a business setting, Hobbs and Nelson [20] use a bilevel program to develop a model for the electric utility industry. At the upper level, the electric utility industry (the leader) seeks to either minimize costs or maximize benefits while controlling electricity rates and subsidizing energy conservation programs. Customers (the followers) attempt to maximize their net benefit by consuming electricity and investing in conservation. This instance is quite small and no details are given for a general solution technique.

As might be expected, many engineering applications require quadratic constraints in order to correctly model natural relationships. Structural design optimization problems, for example, require a mathematical formulation which accurately describes physical laws. In one application, Hajela [19] studied the problem of minimum weight sizing for truss configurations. He found that indeterminate systems required quadratic stress and displacement constraints. Another civil engineering application deals with the planning involved for water distribution systems. Klempous [23] considers an optimal strategy for controlling pumping stations so that consumer demand is met at a minimum cost, while reservoir levels are maintained at a desired level. After making simplifying assumptions, the model which is used minimizes a linear function over a quadratic set of constraints. In this formulation, the quadratic constraint matrices Q_i are indefinite. These constraints relate the number of working pumps, the output flow, and the head of water. The number of these constraints equals the sum of the number of pumping stations and the number of

reservoirs.

Quadratic constraints have proven useful in electrical engineering, especially in the areas of VLSI design and signal processing. A key aspect of VLSI design is the best location of integrated circuits on the circuit board. Eben-Chaime [11] formulated a quadratically constrained reverse convex programming model which can be used to accomplish this difficult task. In this formulation, the quadratic constraints ensure that the various components are placed in non-overlapping locations. In a signal processing design application, Er [13] made use of a quadratic objective and a single quadratic constraint in notch filter design. This formulation allowed his design to accomplish two objectives, achieving one by satisfying the constraint, and the other by minimizing the objective function. Er [14] uses a similar construction (one quadratic objective with one quadratic constraint) to design antennas.

Chemical engineering requires the extensive use of nonlinear programming techniques. Floudas and Visweswaran [16] present a simple pooling problem as an example for which quadratic constraints are required to ensure product quality. In this example, three input streams, each with a unique chemical composition, come together to produce two final products, each of which must meet certain quality standards. Complicating this problem is the fact that two inputs are mixed together in a common pool before combining with the other input to form the final products. The pooling of the two products requires the introduction of both bilinear inequality constraints and bilinear equality constraints. A more complex example, representing an actual application, is also given of a multiperiod tankage quality problem. This program maximizes a linear function which defines total value at the end of the last period over 22 constraints. Of those constraints, 12 were nonconvex bilinear constraints similar to those in the smaller example.

The preceding brief survey is designed to introduce the broad areas of application for the quadratically constrained quadratic program. Certainly in a scientific setting, where models must reflect the true state of reality, the flexibility introduced by the use of nonlinear constraints is often necessary for an adequate description of a problem. While many methods have been used in order to solve programs of this sort, many are not well-suited for larger problem instances. For example, dynamic programming, or any technique which relies significantly on enumeration strategies, will encounter difficulties when used for large problems. In other cases, global optimal solutions are deemed to be too difficult to find and heuristic and dual procedures are used to produce bounds on such a solution. Some applications, especially ones with few constraints, have a structure which allows specialized solution techniques. However, these are often the result of complicated analysis and are not applicable to the broader class of quadratically constrained quadratic programs. We present next a general purpose algorithm for finding global solutions to this class of problems and discuss alternative strategies to accelerate convergence and increase the size of the problems that can be solved in this way.

3 Algorithm

As previously mentioned, solving a quadratically constrained quadratic program is extremely difficult in general. Pardalos and Vavasis [25] have shown that even the simplest linearly constrained nonconvex quadratic program is an NP-hard problem by proving that this holds even when matrix Q_0 is of rank one, with exactly one negative eigenvalue. Of course, the addition of quadratic constraints complicates their problem significantly. Since this problem is inherently hard to solve, a good approach is to find a tractable problem which approximates the original one. The natural

choice for this approximation is a linear program, because of our desire to treat large scale instances of the original problem.

One successful approach along these lines was proposed by Al-Khayyal and Falk [3] and specialized to the quadratic case by Al-Khayyal and Larsen [4]. Sherali and Tuncbilek [28] further extended the procedure to handle all polynomial functions. Adams and Sherali [1] demonstrated that a generalization of this technique could be used to solve quadratic mixed integer programs. This approach provides a conceptually straight-forward method of generating a linear program which approximates the original problem. In the case of a quadratically constrained quadratic program, the LP approximation (or LP relaxation) is formed as follows. The nonlinear terms, which are all the product of two (not necessarily distinct) variables, must be replaced by simple linear ones, each of which represents one of these products. For example, $6x_1^2$ becomes $6w_{11}$ and $3x_1x_2$ becomes $3w_{12}$. Of course, this formulation cannot constrain the new linear terms to equal the product which they represent (i.e. w_{12} cannot be set equal to x_1x_2 , else we would lose the linear programming formulation). However, given bounds on all original variables, it is possible to constrain the new linear terms to be within a well-defined area which envelops the equations $w_{ij} = x_i x_j \forall i, j$. For example, if ℓ_i is a lower bound and u_i is an upper bound such that $\ell_i \leq x_i \leq u_i$, then clearly $(x_i - \ell_i) \geq 0$ and $(u_i - x_i) \geq 0$. Therefore $(x_i - \ell_i)(x_i - \ell_i) = x_i^2 - 2\ell_i x_i + \ell_i^2 \geq 0$, and, using the approximating term, $w_{ii} - 2\ell_i x_i + \ell_i^2 \geq 0$. Similiar constraints may be generated using the upper bound inequality $(u_i - x_i) \geq 0$ and any possible combination of the product of two of these inequalities. The linear constraints constructed in this fashion are called *implied constraints*, and such constraints are frequently studied in integer programming when attempting to characterize a facet of the convex hull of integer points.

To illustrate this procedure, consider the following bilinear program with bilinear constraints:

$$\begin{array}{ll} \text{Min} & 3x + 7y + 4xy \\ \text{subject to} & -7x - 4y - 6xy \leq -50 \\ & -3x - 8y - 5xy \leq -40 \\ & 0 \leq x \leq 15 \\ & 0 \leq y \leq 13 \end{array}$$

The first step in producing the LP approximation program is to replace all nonlinear xy terms with a linear variable, say w . Secondly, bounds on variables x and y are used to limit the allowable values for w . Since $(x-0)(y-0) = xy \geq 0$, w is also constrained by $w \geq 0$. Since $(15-x)(13-y) = 195 - 13x - 15y + xy \geq 0$, w is also constrained by $w - 13x - 15y + 195 \geq 0$. Similarly, w may be constrained from above by combining upper bounds with lower bounds. This results in the two inequalities $(15-x)(y-0) = 15y - xy \geq 0$ and $(x-0)(13-y) = 13x - xy \geq 0$. Hence, w is constrained by inequalities $w - 15y \leq 0$ and $w - 13x \leq 0$. The completed LP is given by

$$\begin{array}{ll} \text{Min} & 3x + 7y + 4w \\ \text{subject to} & -7x - 4y - 6w \leq -50 \\ & -3x - 8y - 5w \leq -40 \\ & w \geq 0 \end{array}$$

$$\begin{aligned}
w - 13x - 15y &\geq -195 \\
w - 15y &\leq 0 \\
w - 13x &\leq 0
\end{aligned}$$

Note that the original bounds no longer need to be explicitly stated. Any solution which satisfies these constraints will also satisfy the original problem's bounds on x and y . For example, since $w \geq 0$ and $15y \geq w$, clearly y must satisfy $y \geq 0$. It is easily shown that original problem bounds must always be similarly satisfied by any feasible solution to the LP relaxation.

When all of the possible implied constraints that can be derived from variable bounds are added to the linearized relaxation of the original constraints, a linear program emerges which has many desirable properties. First of all, the LP relaxation serves as a lower bound for the original nonlinear program since any feasible solution to the original problem is certainly also feasible to the LP. Secondly, if any original variable x_j is at its upper or lower bound at the optimal solution, all approximating variables w_{ij} associated with the product of x_j and any other x_i will exactly equal that product. Finally, the largest possible difference between a linear approximation term w_{ij} and the product $x_i x_j$ which it represents is equal to $\frac{1}{4}(u_i - \ell_i)(u_j - \ell_j)$. Hence, as the distance from each ℓ_j to u_j gets increasingly smaller, w_{ij} will eventually get within any given ε of $x_i x_j$. This convergence provides the motivation for a branch-and-bound optimization algorithm.

The branch-and-bound procedure begins by solving an LP relaxation which includes constraints generated by the bounds given for each variable. If the solution solves the original problem (i.e. each $w_{ij} = x_i x_j$ as well as satisfying all original constraints), the solution is optimal for the original problem. Otherwise the maximum difference $|w_{ij} - x_i x_j|$ is identified. Branching is done to decrease this difference by branching on x_i or x_j . Without loss of generality, assume x_j is chosen and the solution to the first problem has $x_j = s_j$. Two new problems are generated, one of which generates constraints using $\ell_j \leq x_j \leq s_j$ and the other using $s_j \leq x_j \leq u_j$. Clearly, $\ell_j < s_j < u_j$, since if s_j was exactly equal to either ℓ_j or u_j this would imply that each $w_{ij} = x_i x_j$. Hence, each of these problems decreases the maximum possible difference $|w_{ij} - x_i x_j|$. In the example problem given previously, the optimal solution to the LP is found at $x^* = 1.30435, y^* = 0.43478$, and $w^* = 6.52174$. The difference between w and the product xy is 5.9546. In this case, x would be chosen as the branching variable (due to the fact that the optimal x^* was closer to the center of its allowable region than the optimal y^* was). Hence one new problem would be generated using variable bounds $0 \leq x \leq 1.30435, 0 \leq y \leq 13$, and another using $1.30435 \leq x \leq 15$ and $0 \leq y \leq 13$. These problems are solved and further branches are generated in the same fashion.

As the bounds for each variable are tightened, each w_{ij} must eventually get within some acceptable ε of the product $x_i x_j$. When this happens, the LP solution becomes close to feasible for the original problem. This must be true because none of the problem's original constraints are violated by the optimal values of the linear variables w_{ij}^* which are used as substitutes for the actual quadratic terms and each $|w_{ij}^* - x_i^* x_j^*| < \varepsilon$. When the LP solution at any given branch is within an acceptable tolerance of feasibility to the original problem, it must also solve the original problem at that branch. All branches must eventually be fathomed (pruned) for any one of the three reasons: 1) the subproblem of the current node yields a lower bound which is greater than a known feasible solution, 2) the subproblem of the current node is infeasible, or 3) the subproblem of the current node produces a feasible point to the original problem. When all branches have been fathomed, the global solution is the feasible point with the minimum objective value, which resides in one of the branches fathomed for reason (3).

4 Analysis of Algorithm

Certainly the solution procedure detailed above has several desirable properties. First of all, forming the linear relaxations is not difficult either conceptually or computationally. Secondly, the procedure can be shown to converge to a global solution. This property sets this approach apart from many of the traditional, gradient-based approaches for solving nonlinear programs which often converge to points which are only guaranteed to be local solutions. The procedure also generates progressively improving lower bounds.

One of the drawbacks of this procedure is that the size of the LP relaxations can grow exponentially large if all implied constraints are utilized. If a problem has many linear terms, but only a few quadratic ones, the size of the LP will not be much larger than the size of the original problem (in terms of the total number of variables and constraints), if only first level implied constraints are used. When there are many quadratic terms, each distinct nonlinear product $x_i x_j$ is replaced by a new variable w_{ij} . The number of such variables in the LP can be much higher than the original number of variables. In the worst case, if all the possible products of the form $x_i x_j$ are part of a quadratic problem with n variables, then a total of $\frac{n(n+1)}{2}$ additional variables are necessary to linearize each one of these products. To illustrate how fast this enlarges a problem, an original problem has 50 variables, then the could have an LP relaxation with as many as 1275 additional variables.

Perhaps even more important than the additional variables, each new variable which is introduced also requires additional constraints. For a quadratic term of the form $x_i x_j$, where $i \neq j$, if only the first level of implied constraints are used then four new constraints are introduced, which arise from the four inequalities:

$$\begin{aligned} (i) \quad & (x_i - \ell_i)(x_j - \ell_j) \geq 0 \\ (ii) \quad & (x_i - \ell_i)(u_j - x_j) \geq 0 \\ (iii) \quad & (u_i - x_i)(x_j - \ell_j) \geq 0 \\ (iv) \quad & (u_i - x_i)(u_j - x_j) \geq 0. \end{aligned}$$

If $i = j$, then inequalities (ii) and (iii) are identical and hence only 3 new constraints are necessary. Returning to the case where all possible product terms actually occur in the problem, a problem with n variables would generate an LP with $\frac{n(n+1)}{2}$ new variables. The n products of the form $x_i x_i$ require 3 additional constraints, while the rest require 4. Hence, if every possible first level implied constraint is actually generated, an additional $2n(n+1) - n$ constraints are created. If the original problem had 50 variables, the LP may therefore have an additional 5050 constraints. Note that this only considers constraints with first level implied constraints, which can be derived by taking two bound products at a time. Improved linear programming relaxations can be obtained by adding implied constraints derived from bound products taken three at a time, four at a time, all the way up to n at a time. However, this will add an exponential number of constraints and force the use of decomposition and subgradient optimization methods to solve the resultant LP. For this reason, in the procedures developed herein, we shall use only first level implied constraints in the sequel.

A second potential obstacle to be dealt with is the number of branches that are explored before a feasible solution is found. To understand how serious a concern this can be, it is helpful to consider

a simple example. To simplify the analysis, assume that a solution is defined as being feasible if all original constraints are within 0.0001 of being satisfied. Further assume that all original constraints will be satisfied within a tolerance of 0.0001 if each $|w_{ij} - x_i x_j| < 0.000001$. This would in fact be true if each constraint coefficient is < 10 and no more than 10 approximation terms w_{ij} occur in any one original constraint. To see that this holds, note that all constraints are satisfied using the w_{ij} variables. Thus, replacing any w_{ij} variable with the actual $x_i x_j$ product they represent could change the left-hand side of the constraint by no more than 0.00001. Hence, replacing 10 (or fewer) linearized terms with their actual product can cause the constraint to be violated by no more than 0.0001. Recall that the maximum possible difference $|w_{ij} - x_i x_j| = \frac{1}{4}(u_i - \ell_i)(u_j - \ell_j)$. Hence $|w_{ij} - x_i x_j| \leq 0.000001$ if each $u_j - \ell_j \leq 0.001414$. To illustrate the number of branches required to achieve this level of precision, consider an example with only 10 variables, each of which is originally constrained to be between 0 and 40. Assuming that each branch bisects an interval, it would require 32.768 branches to cover the entire interval for any single variable such that each branch satisfies $u_j - \ell_j < 0.001414$. Since this must be done for each variable, upto 327,680 branches could conceivably be created. Hence, even problems with very few variables could, in the worst case, require the solution of an enormous number of LPs.

Of course, in actual problems, good solution areas will be quickly identified and then explored until a feasible solution is found. This allows the algorithm to fathom branches which contain the majority of the original feasible region before any extensive exploration of these regions takes place. Nevertheless, the number of branches involved in exploring these good areas may still be significant.

The power of the branch-and-bound procedure provides a strong motivation for devising methods which reduce potential difficulties due to the number of branches, constraints, and variables. Significant improvements have been made in the overall algorithm by addressing these concerns. We will strive to translate our progress in this area to enhance these methods from having theoretically potential to being practical solution techniques.

5 Improvements

The focus of our research has been to devise methods which start the branch-and-bound procedure with a good, hopefully near-optimal, feasible solution. To be effective this must be done in conjunction with procedures that find tight upper bounds. Together these two algorithmic properties will result in early fathoming of many nodes and thus identify a global optimal solution without an excessive number of branches to establish optimality. For this purpose, heuristic approaches were devised which take advantage of the structure inherent in specific problems. Such techniques proved extremely valuable for finding good feasible solutions with a minimal amount of work, but their effectiveness is highly problem dependent.

To illustrate how effective this approach can be, consider the bilinear program given earlier. By taking advantage of the structure of the problem, a very good solution can be found using the following alternating technique. Initially, set $y^0 = 0$ and solve an LP for the optimal x given $y = y^0$. The solution to this problem is found at $x = 13\frac{1}{3}$. Similarly, solving an LP for y given $x^0 = 0$ yields the solution $y = 12\frac{1}{2}$. We now assume that a good solution is very likely to lie in the region $0 \leq x \leq 13\frac{1}{3}$, $0 \leq y \leq 12\frac{1}{2}$. Thus, an LP relaxation is generated using these bounds and an optimal solution is found at $x^1 = 1.37931$, $y^1 = 0.48030$. This solution is not feasible, so we continue by once again solving two LPs: one for the optimal x given $y = y^1$ and one for the optimal y given $x = x^1$. The solutions to these LPs ($x = 6.6940$ and $y = 3.2865$, respectively) are then used to provide bounds for

another LP approximation problem. Once again, the heuristic is based upon the likelihood of a good solution being in the region $1.37931 \leq x \leq 6.6940$, $0.48030 \leq y \leq 3.2865$. Following the example to its conclusion, the solution to this LP relaxation is infeasible point $x^2 = 2.43094$, $y^2 = 1.03557$. Linear programs for x given $y = y^2$ and for y given $x = x^2$ yield the bounds $2.43094 \leq x \leq 3.8782$, $1.03557 \leq y \leq 1.7747$. Solving a third linear relaxation yields $x^3 = 2.85227$, $y^3 = 1.37459$, which in turn generates LPs which provide bounds $2.85227 \leq x \leq 2.93765$, $1.37459 \leq y \leq 1.4225$. Given these much tighter bounds, the solution $x^4 = 2.88794$, $y^4 = 1.39625$ yields a point which is very near feasible. The heuristic therefore concludes by solving two final LPs (one for y given $x = x^4$ and one for x given $y = y^4$) and using the better of the two solutions as an upper bound. In this case, the solution $x = 2.88842$, $y = 1.39625$ provides an excellent upper bound of 34.57084 on the objective function. To see how good this bound is, we note that the actual optimal solution $x = 2.88814$, $y = 1.39637$ has objective function value of 34.5707. Clearly, the success of the above approach was highly correlated to the size of the problem and the bilinear structure of the functions. However, the example illustrates the potential of fully exploiting problem structure, even for NP-hard problems.

In the previous example, the heuristic worked especially well for several reasons. First, the objective function was monotonically increasing as a function of either x or y . Similarly, the left-hand side of the constraints was monotonically decreasing as a function of either x or y . Finally, the problem was tractable given initial values $x^0 = 0$ and $y^0 = 0$.

When problem structure does not easily give rise to specialized algorithms, as in the bilinear case above, we investigated other techniques that were based on the use of infeasible solutions that are generated by the LP relaxation. As the variable bounds which generated the linear relaxations become increasingly small, the optimal solutions to these approximating problems approach the feasible set. Hence, it is reasonable to use these solutions as starting points, and then move in a search direction which seems likely to quickly intersect the feasible region. One method of accomplishing this is illustrated on the following problem:

$$\begin{array}{ll}
\text{Min} & 11x_1 + 9x_2 + 7y_1 + 12y_2 + 3x_1y_1 + x_2y_2 + 4x_2y_1 + 2x_2y_2 \\
\text{subject to} & -5x_1 - 8y_1 - 7x_1y_1 - 3x_1y_2 + 2x_2y_1 - 9x_2y_2 \leq -70 \quad (1) \\
& -8x_2 - 10y_2 + 6x_1y_1 - 8x_1y_2 - 5x_2y_1 - x_2y_2 \leq -40 \quad (2) \\
& -2x_1 - 3x_2 - y_1 - 5y_2 - 3x_1y_1 + 2x_1y_2 - 7x_2y_1 - 2x_2y_2 \leq -50 \quad (3) \\
& x_1 - 6x_2 - 5y_1 - 8x_1y_1 - x_1y_2 + x_2y_1 - 6x_2y_2 \leq -60 \quad (4) .
\end{array}$$

This problem was solved by the branch and bound method without any enhancements and required the solution of LP relaxations at 160 branches to attain the desired solution accuracy. As an example of an LP relaxation which yields a good near-feasible solution, branch number 114 (of the 160 branches) solves the LP generated by the following bound constraints.

$$0 \leq x_1 \leq 10, 3.1428 \leq x_2 \leq 3.1472, 0.1850 \leq y_1 \leq 0.5783, 2.0788 \leq y_2 \leq 10$$

The solution to this LP relaxation is

$$x_1 = 0, x_2 = 3.1430, y_1 = 0.5666, y_2 = 2.4398,$$

with an objective function value of 83.9939. It is easily demonstrated that this solution satisfies constraints 2 and 4, but slightly violates constraints 1 and 3.

Clearly, if only one constraint was violated, an effective method for finding a point which satisfies that constraint would be to move in the direction of steepest descent (i.e. the negative gradient) of the constraint function until that constraint is satisfied. When multiple constraints are violated, a direction must be found which tends to reduce all such constraints. Therefore, the negative gradients of all the violated constraints are useful for identifying a direction which points towards the region where all of these constraints are satisfied. A promising direction would lie within the cone formed by all of these negative gradients. A logical choice is to search in the direction obtained by averaging all of these negative gradient directions, although more complicated procedures could also be used to find directions which were more centrally located within this cone. In our example, the normalized negative gradients of constraints 1 and 3 are

$$\begin{aligned} g_1(x, y) &= (0.4202, 0.5374, 0.0442, 0.7299)^T \text{ and} \\ g_3(x, y) &= (-0.0418, 0.4193, 0.8142, 0.3995)^T. \end{aligned}$$

Thus, a reasonable search direction would be the average of these two directions, which is

$$d(x, y) = (0.1892, 0.4783, 0.4292, 0.5647)^T$$

Moving even a small distance in this direction does in fact yield a feasible point. In this case, letting $x_{new} = x_{old} + \lambda d$ where $\lambda = 0.000469$ yields a feasible point (x, y) with an objective function value of 84.0045. The objective function value associated with this feasible point differs from the objective function value of the optimal solution to the LP relaxation at that branch by only 0.0106. Hence, the feasible solution yields a tight upper bound which allows several branches to be fathomed. Techniques which take advantage of the information provided by the LP relaxations, as this one does, are very effective if they are designed to be computationally simple and have a high probability of being successful. The latter property is highly problem dependent.

Finding good upper bounds, as described above, is only one-half of a total strategy to accelerate convergence. The second half calls for finding good lower bounds on the global optimal objective value for each subproblem. Solving the LP approximation problems is method of providing lower bounds. However, in the early stages of the branch-and-bound algorithm, when variable bounds are somewhat loose, the lower bounds produced are not in general tight enough to contribute to fathoming. Problem specific heuristics (in the spirit of the one detailed above for finding tight upper bounds) for improving lower bounds for promising subproblems region were investigated. The most robust strategy involved solving the Lagrangian dual of a tractable relaxed problem. For example, given the variable bounds at a certain branch, an effective method of finding a lower bound on the objective function over the subproblem's feasible set would be to consider the augmented Lagrangian function. For a problem of the form

$$\begin{aligned} \text{Min} \quad & f(x) \\ \text{subject to} \quad & g(x) \leq 0, \end{aligned}$$

the Lagrangian function is defined for $u \geq 0$ by

$$\Theta(u) = \inf_x (f(x) + u^t g(x)).$$

The augmented Lagrangian function is created by augmenting the original objective function with terms which penalize the violation of the problem's constraints, and then defining the Lagrangian function as above based on the augmented objective function. The value of the augmented Lagrangian function for any given vector u of Lagrange multipliers provides a lower bound on the optimal value of $f(x)$. Unfortunately, finding this lower bound may require considerable effort in some instances. However, within the context of the branch-and-bound algorithm, minimizing the Lagrangian function may be efficient and useful. The reason for this is that the branch-and-bound algorithm produces a solution which in general would tend to be close to the actual optimal solution for the variable bounds at a given branch. Thus, starting from this near-optimal point would allow faster convergence to the true solution than starting from some arbitrary point. Secondly, the branch-and-bound algorithm could be helpful in providing Lagrange multipliers which are close to the optimal multipliers. Hence, the value of $\Theta(u)$, where u is obtained from the solution of the relaxed linear programming problem in the branch-and-bound algorithm, should be close to the value of $\Theta(u^*)$, where u^* is the vector of optimal Lagrange multipliers, whenever u is close to u^* . Moreover, $\Theta(u)$ serves as a lower bound on the subproblem's optimal objective value and this lower bound is better (higher) than that obtained from the linear programming relaxation.

Another way of improving the lower bounds is to tighten the approximation of the LP relaxations by adding more implied constraints. Research into methods for identifying the critical implied constraints that improve the lower bounds found at each branch is ongoing and no conclusive results are ready for dissemination at this time. Another interesting ongoing research area is the identification of either redundant constraints or constraints that tighten the feasible region's approximation too far away from the neighborhood of an optimal solution to do any good. In this way tight LP relaxations can be made small enough to be solvable by standard algorithms, without the need to resort to large-scale methods such as subgradient optimization or successive over-relaxation. The idea of dropping implied constraints that tighten the region far from an optimal solution was very effective on the location problems studied by Sherali and Tuncbilek (1992). In that work, the authors applied analytical techniques to the plant location problem in their attempt to reduce the number of additional constraints generated to form the LP relaxation. They determined that the constraints generated by multiplying $(u_i - x_i)(u_j - x_j)$ could be ignored without causing a significant difference in the value of the optimal solution to the LP. This result is not surprising for the location problem since the constraints that were dropped formed lower bounds on linear approximation variables that the objective function sought to maximize. Since the optimization process attempted to increase the value of these variables, the lower bounds induced by such implied constraints were rarely active at an optimal solution to the relaxed problem.

Most branching tends to occur in those regions which in fact contain good solutions. Thus, a natural method of improving the overall algorithm would be to use a two step approach: 1) use the branch-and-bound procedure to identify areas which are likely to contain good solutions, and 2) use a rapidly convergent technique in order to find a local solution in the area of interest. Several traditional nonlinear programming techniques are available to accomplish this second step. Initial testing of this idea was done using Newton's method for solving systems of nonlinear equations.

To illustrate its effectiveness in the context of a branch-and-bound algorithm, consider our bi-linear example. In this implementation, Newton's method for solving simultaneous equations is attempted only when the maximum difference $|w_{ij} - x_i x_j|$ is less than a given distance. We assume that the set of near binding constraints at the node's LP approximate solution are active at a local solution. In this example, Newton's method is first attempted at branch 15, which

has LP solution $x = 2.56774, y = 1.08904, w = 4.71690$. Neither constraint is satisfied with $x = 2.56774, y = 1.08904$, hence we seek to find a solution by using Newton's method for solving four simultaneous equations. Two equations come from assuming both inequality constraints will be tight at a solution, the other two equations come from setting the partial derivatives of the Lagrangian with respect to both x and y equal to zero, which corresponds to a first order necessary condition holding at the local solution. After 3 iterations, Newton's method converges to $x = 2.88814, y = 1.39637$, and Lagrange multipliers $u = (0.05655, 0.77299)^T$. This is in fact the optimal solution to the original problem and the branch-and-bound algorithm is completed after 21 branches. Using the unenhanced version of the branch-and-bound procedure, 57 branches were required to solve the problem. Similar results have been achieved for slightly larger problems. Larger problems may require more sophisticated algorithms both for finding local solutions and for identifying when branches may be fathomed. Research is ongoing to explore these techniques in order to find methods which converge consistently and also quickly. Ideally, the combination of the global search inherent in the branch-and-bound algorithm and the rapid local convergence of traditional nonlinear methods should result in a powerful and efficient algorithm.

Instead of solving smaller relaxed linear programs, faster Lagrangian methods can be used to solve the large scale LPs that are generated at each branch of the branch-and-bound tree. Tunchilek (1992) considers a Lagrangian approach to solving a quadratic program with only linear constraints. In this approach, all original constraints are moved into the objective function. Quadratic terms x_i^2 are allowed to remain in the objective function. On the other hand, cross-product terms of the form $x_i x_j$ are simply replaced with either a linear over or under estimate (depending on their objective function coefficient) derived from bound products. Hence no additional bound product constraints or additional variables w_{ij} are required. The resulting subproblem is therefore considerably smaller. Also, given any vector of Lagrange multipliers, the subproblem is separable and reduces to minimizing n quadratic functions over a bounded interval which is easy to solve. This allows for an exceptionally efficient solution of the Lagrangian subproblem at each step. Substituting linear functions for all cross-product terms, while greatly reducing the work required to solve a particular problem, also tends to lessen the quality of the lower bound produced by this algorithm. We have extended this idea to the quadratically-constrained problem and have begun testing its effectiveness on small problems. We are still in the process of delineating conditions and problem properties under which this Lagrangian technique is worthwhile. We will continue to explore methods for calculating lower bounds as part of a branch-and-bound approach to much larger problems.

6 Impact and Future Research

The global optimization algorithm previously discussed is attractive both because it is powerful and because it is easy to understand and implement for a wide variety of applications. The basic algorithm has been published in [5] and the preliminary results on its enhancements are reported in [36]. Our research paves the way for allowing this algorithm to become a practical method for solving Operations Research problems encountered in real-world situations. In order to reach this goal, further research discoveries need to be made which will alleviate the difficulties associated with the size and number of linear relaxations which must be solved in the course of using this approach.

To fully explore the potential of some of the ideas developed in this research effort, fast nonlin-

ear programming techniques need to be fully integrated into a global branch-and-bound algorithm. (We have only validated the efficacy of using these approaches on a limited set of test problems.) Bringing these two techniques together in a working code will allow for extensive numerical experimentation to establish how effective the overall procedure is on a wide range of problems.

Exploiting problem structure to gain a better understanding of the linear relaxations formulated at each branch of the branch-and-bound tree will lead to more efficient methods of solving these problems. In particular, generating only those implied constraints that improve the quality of the lower bound will significantly reduce the size of the subproblems to be solved. Also, Lagrangian dual techniques, which are frequently used to solve large linear programs, have been shown by others [29] to generate useful lower bounds for certain location problems.

Other advances can be made by developing powerful techniques for finding near-optimal feasible points for use as upper bounds. An efficient method for finding good feasible solutions to nonlinearly constrained problems, starting from nearby infeasible points, is by itself a worthy goal. Any discoveries along these lines will both increase the theoretical understanding of nonlinear programming problems and improve the performance of existing algorithms.

A promising new technique for solving the class of problems under investigation is based on decomposing each function into the difference of two convex (*d.c.*) functions. This gives rise to a *d.c. optimization problem* which can be solved by either a branch-and-bound technique or an outer-approximation technique. Tuy *et al* [35] have successfully specialized the general approach to the solution of large-scale single facility location problems with both attraction and repulsion. Refinement of this procedure will be studied using a *new* *d.c.* decomposition of quadratic functions. Completion of the research will produce a new algorithm for global optimization of “large” quadratically constrained problems.

7 List of Publications

The following publications acknowledge NSF Grant DMII-91-14489 as a partial supporter of the research effort entailed in their preparation. The results in [27] helped to understand and explain in which situations local procedures will converge finitely.

- Al-Khayyal, F.A., Larsen, C., and T. Van Voorhis (1995), A relaxation method for nonconvex quadratically constrained quadratic programs, *Journal of Global Optimization* **6**, 215-230.
- Shapiro, A., and F. Al-Khayyal (1993), First-order conditions for isolated locally optimal solutions, *Journal of Optimization Theory and Applications* **77**, 189-196.
- Sherali, H.D., Krishnamurthy, R.S., and F.A. Al-Khayyal (1996), Enhanced intersection cutting plane approach for linear complementarity problems, *Journal of Optimization Theory and Applications*, to appear.
- Tuy, H., Al-Khayyal, F.A., and F. Zhou (1996), A *d.c.* optimization method for single facility location problems, *Journal of Global Optimization*, to appear.
- Van Voorhis, T., and F.A. Al-Khayyal (1995), Accelerating convergence of branch and bound algorithms for quadratically constrained optimization problems, in *State of the Art in Global Optimization: Computational Methods and Applications*, C.A. Floudas and P.M. Pardalos, eds., Kluwer Academic Publishers, Boston, to appear.

- Van Voorhis, T.P., (1996), Algorithms for indefinite quadratically constrained quadratic programs, Ph.D. Dissertation, School of Industrial and Systems Engineering, Georgia Institute of Technology, Atlanta, Georgia, 30306-0205. in preparation.

In addition, papers in preparation that *will* acknowledge NSF Grant DMII-91-14489 include the following.

- ♣ A linearization relaxation technique for linear complementarity problems (with H.D. Serali and R.S. Krishnamurthy).
- ♣ A d.c. optimization method for multifacility location problems (with H. Tuy and F. Zhou).
- ♣ A d.c. optimization technique for quadratically constrained quadratic programs (with T. Van Voorhis).
- ♣ On finitely terminating branch-and-bound algorithms for some global optimization problems (with H.D. Serali).

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