Solution of Contact Problems Using Subroutine BOX-QUACAN*

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Abstract
An augmented Lagrangian type algorithm, specifically designed for strictly convex quadratic programming problems with simple bounds and linear equality constraints is described. The main feature of this algorithm is the precision control of the auxiliary problems, that are solved using the subroutine BOX-QUACAN *developed at the University of Campinas. The main algorithm was used to solve contact problems of elastic bodies.*

Keywords: Quadratic programming, Augmented Lagrangian, Contact problems.

1 Introduction

We will be concerned with the problem of finding a minimizer of a function subject to simple bounds and linear equality constraints (SBE), that is

$$\begin{array}{ll} \text{Minimize} & q(x) \\ \text{subject to} & x \in \Omega \end{array} \tag{1}$$

with $\Omega = \{x \in \mathbb{R}^n \mid x \geq 0 \text{ and } Cx = d\}$, $q(x) = \frac{1}{2}x^T Ax - b^T x$, $b \in \mathbb{R}^n$, $d \in \mathbb{R}^m$, $A \in \mathbb{R}^{n\times n}$ symmetric positive definite, and $C \in \mathbb{R}^{m\times n}$ a full rank matrix. We are

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especially interested in problems with m much smaller than n and with the matrix A large and reasonably conditioned (or preconditioned), so that conjugate gradient based methods are directly applicable. Such problems arise, for example, from the discretization of the variational inequality that describes the equilibrium of a system of elastic bodies in contact in reciprocal formulation whenever such system includes floating bodies (e.g. Hlaváček et al. [21], Dostál [7, 6, 8]).

The problem of identifying contact interfaces and evaluation of strain contact stresses of systems of elastic bodies in contact is modelled by the discrete reciprocal formulation obtained by the symmetric boundary element method. The details of the modelling and the reduction of the original problem to a sequence of strictly convex quadratic programming problems subject to simple bounds are discussed in [9].

The problem of modelling a system of deformable blocks is the subject of [11], where the equilibrium conditions of the block system are described by a discretized variational inequality, that is reduced by duality to a sequence of convex quadratic programming problems with simple bounds. In both articles [9, 11], domain decomposition techniques for solving these problems are discussed. The formulation of the problems obtained in [9, 11] is typical for a large class of problems arising in mechanical engineering.

While in [9, 11] we emphasized modelling and formulation of the problems, in the present paper implementation issues are the main subject. A description and some details of the implementation of the algorithm and the way the package `BOX-QUACAN` is used may be of interest for potential users of this software, that is available for free under request. The authors are interested in testing the performance of this software with other problems.

We shall restrict our attention to algorithms that reduce problem (1) to a sequence of quadratic programming problems with simple bounds. Our approach has been motivated by the need of efficient algorithms for solving the problems mentioned above and recent progress in the solution of problem (1), such as effective exploitation of projections (e.g. Moré and Toraldo [22]) that allows drastic changes in the active set from one iteration to another, and results of the present authors [1, 6, 7, 10, 12, 13, 14] that enable to adaptively control the precision of the solution of auxiliary problems while preserving qualitative properties of the already known algorithms.

Our starting point is the algorithm presented by Conn, Gould and Toint [2] who adapted the augmented Lagrangian method of Powell [23] and Hestenes [19] to the solution of problems with a general cost function subject to general equality constraints and simple bounds. When applied to (SBE), their algorithm reduces it to a sequence of simple bound constrained problems (SB)

$$\begin{array}{rl} \text{Minimize} & L(x, \mu^k, \rho_k) \\ \text{subject to} & x \geq 0 \end{array}$$

where

$$L(x, \mu^k, \rho_k) = q(x) + (\mu^k)^T (Cx - d) + \frac{\rho_k}{2} \|Cx - d\|^2$$

is known as the Lagrangian function, $\mu^k = (\mu_1^k, \ldots, \mu_m^k)^T$ is the vector of Lagrange multipliers for equalities, ρ_k is the penalty parameter, and $\|\cdot\|$ denotes the Euclidian norm. These authors developed basic methods of analysis, proved convergence results that cover also the possibility to exploit inexact solutions of (SB), and established that a potentially troublesome penalty parameter is bounded. They implemented their algorithm in the successful package `LANCELOT` [3].

The main improvement that we propose on the algorithm of Conn, Gould and Toint concerns the control of precision of the solution of the auxiliary problem (SB). Our approach arises from the simple observation that the precision of the solution x^k of the auxiliary problem (SB) should be related to the feasibility of x^k, i.e. $\|Cx^k - d\|$, since it does not seem reasonable to solve (SB) with high precision when μ^k is far from the Lagrange multiplier of the solution of (SBE). The present paper is divided in five sections. In Section 2 we describe the algorithm and comment on its theoretical properties, that were proved in [10]. In Section 3 we discuss its implementation and in Section 4 we report on computational experiments with contact problems. Finally, in Section 5 some conclusions are presented.

The following notations and definitions will be used. The gradient of the augmented Lagrangian will be denoted by g, so that

$$g(x, \mu, \rho) \quad = \quad \nabla_x L(x, \mu, \rho) \quad = \quad \nabla q(x) + C^T \mu + \rho C^T (Cx - d)$$

The Karush-Kuhn-Tucker (KKT) conditions for problem (SB) may be conveniently described by the projected gradient g^P that is defined by

$$\begin{array}{rcl} g_i^P & = & g_i \quad \text{if} \quad x_i > 0 \quad \text{or} \quad x_i = 0 \quad \text{and} \quad g_i < 0 \\ g_i^P & = & 0 \quad \text{otherwise, i.e.} \quad x_i = 0 \quad \text{and} \quad g_i \geq 0, \end{array}$$

where $g = g(x, \mu, \rho) = (g_1, \ldots, g_n)^T$. Thus the KKT conditions for problem (SB) are satisfied at x if and only if $g^P(x, \mu^k, \rho_k) = 0$.

The chopped gradient g^C, used in [1] and [6], is defined as follows

$$\begin{array}{rcl} g_i^C & = & g_i \quad \text{if} \quad x_i = 0 \quad \text{and} \quad g_i < 0 \\ g_i^C & = & 0 \quad \text{otherwise.} \end{array} \tag{2}$$

Given a point x and the set $J = \{i \in \{1, 2, \ldots, n\} \mid x_i \neq 0\}$, let $C_J \in I\!R^{m \times p}$, with $p \geq m$, be a sub-matrix of C consisting of the columns with indices in J. If C_J is full rank we say that x is *feasibly regular* or briefly *f-regular*.

2 Algorithm for Equality and Simple Bound Constraints

The following algorithm for the solution of (SBE) follows the structure of algorithms of Conn, Gould and Toint [2]. However, as we are dealing with quadratic programming, we introduce some special features as adaptive precision control in Step 1, application of simple penalty to deal with iterations that are not f-regular, and unconditional update of Lagrange multipliers for the f-regular iterations.

Algorithm 1. Given $\eta_0 > 0,\ 0 < \alpha < 1,\ \beta > 1, M > 0,\ \rho_0 > 0,\ \nu > 0,\ \mu^0 \in I\!R^m$ and the matrices and vectors that define problem (1), set $k = 0$.

Step 1. {Inner iteration with adaptive precision control.}
Find z such that

$$\|g^P(z, \mu^k, \rho_k)\| \leq M\|Cz - d\|. \tag{3}$$

Step 2. {Grant small projected gradient for z not f-regular.}
If z is not f-regular, find z such that

$$\|g^P(z, \mu^k, \rho_k)\| \leq \min\{\rho_k^{-\nu}, M\|Cz - d\|\}. \tag{4}$$

Step 3. Set $x^k = z$.

Step 4. {Update μ, ρ, η. }
If x^k is f-regular then

$$\mu^{k+1} = \mu^k + \rho_k(Cx^k - d).$$

If $\|Cx^k - d\| \leq \eta_k$ then

$$\rho_{k+1} = \rho_k, \quad \eta_{k+1} = \alpha\eta_k$$

else

$$\rho_{k+1} = \beta\rho_k, \quad \eta_{k+1} = \eta_k.$$

If x^k is not f-regular then

$$\mu^{k+1} = \mu^k, \quad \rho_{k+1} = \beta\rho_k, \quad \eta_{k+1} = \eta_k.$$

Step 5. Set $k = k + 1$ and return to the Step 1.

In Steps 1 and 2 we can use any algorithm for minimizing a bound constrained quadratic such that the projected gradient converges to zero. Algorithms of this type are presented in [1, 8, 12, 14].

In [10] it is proved that any convergent algorithm for the solution of the auxiliary problem (SB) that is required in Step 1 or Step 2 will generate either z that satisfies (3) or (4) in a finite number of steps or a sequence of approximations that converges to the solution of (1). In particular, this shows that there is no hidden enforcement of exact solution in conditions (3) and (4).

Algorithm 1 has been proved to converge for any set of parameters that satisfy the prescribed relations. Moreover, it has been proved that the asymptotic rate of convergence is the same as for the algorithm with exact solution of the auxiliary quadratic programming problems (i.e. $M = 0$). The penalty parameter has been proved to be uniformly bounded. The proofs of these theoretical properties are in [10].

Algorithm 1 deals separately with each type of constraint and accepts inexact solutions of the auxiliary simple bound constrained problems in Step 1 with the precision proportional to the unfeasibility measure of the current point.

3 Implementation

A version of Algorithm 1 has been implemented in double precision `Fortran 77`. The quadratic programming problems in Steps 1 and 2 are solved using the subroutine `BOX- QUACAN`, developed at the University of Campinas. A brief description of this subroutine and some comments on specializations needed to be used for solving problem (SBE) are the contents of this section. Subroutine `BOX-QUACAN` may be used to solve the following nonlinear programming problem

$$\begin{array}{rl} \text{Minimize} & \phi(x) \\ \text{subject to} & h(x) = 0 \\ & Cx = d \\ & l \leq x \leq u. \end{array} \tag{5}$$

where $\phi : I\!R^n \to I\!R$ is a general nonlinear function, $h : I\!R^n \to I\!R^p$ defines the nonlinear constraints and any component of the bounds l, u may be infinite.

`BOX-QUACAN` implements a trust-region based algorithm that solves any simple bounded problem. Problem (5) might be solved by the augmented Lagrangian approach, that is, given the values ξ and ρ of the penalty parameters and the vectors λ and μ of Lagrange multipliers, `BOX-QUACAN` solves the following simple bounded problem:

$$\begin{array}{rl} \text{Minimize} & \mathcal{L}(x) \\ \text{subject to} & l \leq x \leq u, \end{array} \tag{6}$$

where

$$\mathcal{L}(x) = \phi(x) + \lambda^T h(x) + \frac{\xi}{2}\|h(x)\|_2^2 + \mu^T(Cx - d) + \frac{\rho}{2}\|Cx - d\|_2^2 + \frac{\delta}{2}\|x - x_c\|_2^2.$$

The function $\mathcal{L}$ is the classical augmented Lagrangian for the equality constraints of (5) plus a quadratic regularization term (δ is the regularizing parameter and x_c is a conveniently chosen point).

The method used to solve (6) is described in [14]. At each iteration of `BOX-QUACAN` a quadratic approximation of $\mathcal{L}$ is considered and this quadratic problem is minimized inexactly subject to simple bound constraints. The quadratic approximation does not need to be convex. The quadratic solver `QUACAN` produces an approximation to the solution such that the two-norm of the projected gradient of the quadratic model is as small as desired. Subroutine `QUACAN` implements a matrix-free method based on a mild active set strategy that uses conjugate gradients inside the faces, projected searches and chopped gradients to leave the faces. The method blends results obtained independently in [1] and [6]. The directions used to leave faces enable the finite identification of the correct constraint set even for dual degenerate problems.

The problems we are interested in solving have the structure of (1), being a particular case of (5). The objective function q is quadratic and there are only linear constraints.

In [9, 11] the authors show that the matrix of the resulting quadratic function is BA^+B^T, where $B \in I\!R^{r\times n}$ describes the incremental non-interpenetration condition and A is a symmetric positive semidefinite block diagonal matrix of order n, that is, $A = diag(A_1,\ldots,A_p)$ and A^+ is a generalized inverse of A satisfying $A = AA^+A$. The unknown variables in this formulation are the nodal forces (see [9, 11] for details). The blocks $A_1,\ldots,A_p$, correspond to a domain decomposition of the region Ω into subdomains $\Omega_1,\ldots,\Omega_p$. The blocks A_i are all banded matrices. The number of linear constraints in this formulation is much less than the order of the matrix A.

The heart of the matrix-free approach of `BOX-QUACAN` is the matrix-vector product involving BA^+B^T. Therefore, special care was taken in writing the code for the subroutine that calculates this product. Matrices $A_1,\ldots,A_p$ are stored with banded structure and a band Cholesky factorization, see [18], is used. The factors obtained are saved in the memory positions corresponding to the matrices $A_1,\ldots,A_p$, by overwriting them at the beginning of the process. Once the triangular banded solvers and the action of matrices B and B^T on a vector are coded, given $u \in I\!R^r$, the product $v = BA^+B^Tu$ is calculated by the sequence $y = B^Tu, z = A^+y, v = Bz$. The simple bound quadratic solver `QUACAN` is considered as a black-box managed by `BOX`, the trust-region code for simple bounded nonlinear programming problems. The algorithm introduced in [10] modifies the augmented Lagrangian approach taking advantage of the special structure of the quadratic problems of interest. In these problems f-regularity is satisfied at each iteration. It has been proved in [10] that if the solution of (1) is f-regular, then after a finite number of iterations every current point is also f-regular. In the problems under consideration the dimension m is much smaller than n (typically, $m \le 4$), so that the computational effort to check f-regularity is negligible. The main improvement of our approach is the adjustment of the precision required for approximately solving the auxiliary problems before calling the quadratic solver `QUACAN`. Different intermediate problems (SB) are defined according to the values of the penalty parameters and Lagrange multipliers and then `BOX-QUACAN` is called for solving them.

4 Numerical Experiments

In this section, we illustrate the practical behavior of our algorithm. First, a model problem used to validate the algorithm is presented. Next, two problems arising in mechanical and mining engineering, respectively, are commented. All the experiments were run in a PC-486 type computer, DOS operating system, Microsoft `Fortran 77` and double precision.

Problem 1. This is a model problem resulting from the finite difference discretization of the following continuous problem:

$$\begin{array}{rl}\text{Minimize} & q(u_1,u_2)=\sum_{i=1}^{2}\left(\int_{\Omega_i}|\nabla u_i|^2 d\Omega-\int_{\Omega_i}Pu_i d\Omega\right)\\ \text{subject to} & u_1(0,y)\equiv 0 \text{ and } u_1(1,y)\le u_2(1,y) \text{ for } y\in[0,1],\end{array}$$

where $\Omega_1=(0,1)\times(0,1)$, $\Omega_2=(1,2)\times(0,1)$, $P(x,y)=-1$ for $(x,y)\in(0,1)\times[0.75,1)$, $P(x,y)=0$ for $(x,y)\in(0,1)\times(0,0.75)$, $P(x,y)=-1$ for $(x,y)\in(1,2)\times(0,0.25)$ and $P(x,y)=0$ for $(x,y)\in(1,2)\times(0.25,1)$. The discretization scheme consists in a regular grid of 21×21 nodes for each unitary interval. We took the identically zero initial approximation. This problem is such that the matrix of the quadratic function in (1) is singular due to the lack of Dirichlet data on the boundary of Ω_2. In order to reduce the residual to 10^{-5}, three (SB) problems had to be solved. The total number of iteration used by `QUACAN` was 23, taking 34 matrix-vector products. More details on this problem may be found in [6].

Problem 2. The objective of this problem is to identify the contact interface and evaluate the contact stresses of a system of elastic bodies in contact. Some rigid motion is admitted for these bodies. This type of problems is treated in [9]. The model problem considered to test our algorithm consists of two identical cylinders that lie one above the other on a rigid support. A vertical traction is applied at the top 1/12 of the circunference of the upper cylinder. This problem was first considered admitting vertical rigid motion of the upper cylinder only. A second formulation admitted rigid body motion of both cylinders. The Lagrange multipliers of the solution are the contact nodal forces. To solve the problem with relative precision equal to 10^{-4}, three (SB) problems were solved with $\rho=10^6$, $M=10^4$ and $\Gamma=0.1$. The total number of `QUACAN` iterations was 42.

Problem 3. Finally, we consider a problem of equilibrium of a system of elastic blocks. This problem arises in mining engineering. An example of the solution of such problems under the assumption of plane strain may be found in [4]. The difficulties related to the analysis of equilibrium of block structures comprise identification of unknown contact interface, necessity to deal with floating blocks that do not have enough boundary conditions and often large matrices that arise from the finite element discretization of 3D problems. To test the performance of our algorithm we solved a 3D problem proposed by Hittinger in [20]. The 2D version of this problem was solved in [20] and [5]. A description of the problem and the variants solved with our algorithm are in [11]. A relative precision of 10^{-4} was obtained in all cases with no more than three outer iterations, that is, just three (SB) problems were necessary. The largest number of `QUACAN` iterations was 276.

5 Final Remarks

The problem of minimizing simple bound constrained functions has been extensively studied by many authors. Friedlander, Martínez and Santos [14] developed a trust-region type algorithm for such problems that uses quadratic subproblems. This algorithm was implemented in the subroutines `BOX-QUACAN`, available at the University of Campinas. This subroutine was extensively used to solve convex optimization, complementary problems and variational inequalities [15, 16, 17]. Independently, Dostál [8] developed an algorithm for solving quadratic functions subject to simple bound constraints motivated by physical problems with applications in mining and mechanical engineering. These problems are very challenging and, with the modifications introduced to be used in the context of strictly convex quadratic programming problems with simple bounds and linear equality constraints, `BOX-QUACAN` solved them with a highly encouraging performance. It is worthwhile stressing that all the results were obtained, even those for the 3D problems, using a quite modest equipment. More tests on real problems of the type discussed here are intended to confirm `BOX-QUACAN` as an efficient tool for these applications.

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