BOX-QUACAN and the implementation of Augmented Lagrangian algorithms for minimization with inequality constraints

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Abstract

BOX-QUACAN is a trust-region box-constraint optimization software developed at the Applied Mathematics Department of the University of Campinas. During the last five years, it has been used for solving many practical and academic problems with box constraints and it has been incorporated as sub-algorithm of Augmented Lagrangian methods for minimization with equality constraints and bounds. In this paper it is described its use in connection with Augmented Lagrangian algorithms where inequality constraints are handled without the addition of slack variables. Numerical experiments comparing a modified exponential Lagrangian method and the most classical Augmented Lagrangian are presented.

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Resumo BOX-QUACAN é um software para minimização em caixas baseado em regiões de confiança, desenvolvido no Departamento de Matemática Aplicada da UNICAMP. Durante os últimos cinco anos, tem sido usado para resolver muitos problemas práticos e acadêmicos com restrições de canalização e foi incorporado como sub-algoritmo de métodos de Lagrangeano aumentado para minimização com restrições de igualdade e limitantes. Neste artigo, descreve-se seu uso em conexão com algoritmos de Lagrangeano aumentado, onde as restrições de desigualdade só tratadas sem acrescentar variáveis de folga. São apresentados experimentos numéricos, comparando uma forma modificada del método exponencial Lagrangeano, e o Lagrangeano aumentado mais clássico.

Keywords: Optimization, algorithms, Augmented Lagrangians, Box-constrained minimization.

Palavras chave: Otimização, algoritmos, Lagrangeanos aumentados, minimização em caixas.

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1 Introduction

Box constrained optimization is a well developed area of numerical analysis. It consists on the minimization of a (generally smooth) function subject to bounds on the variables. On one hand, many practical problems have the box-constraint structure. On the other hand, this problem is much easier to solve than the general constrained optimization problem and, for this reason, it is used as subproblem by algorithms that minimize functions with general linear or nonlinear constraints. Progress in the development of box-constraint algorithms has an immediate multiplicative effect on the whole area of nonlinear programming.

BOX-QUACAN is a box-constraint solver whose basic principles are described in [19]. It is an iterative method which, at each iteration, approximates the objective function by a quadratic and minimizes this quadratic model in the box determined by the natural constraints and an auxiliary box that represents the region where the quadratic approximation is reliable (trust region). If the objective function is sufficiently reduced at the (approximate) minimizer of the quadratic, the corresponding trial point is accepted as new iterate. Otherwise, the trust region is reduced. The main algorithmic difference between this method and LANCELOT (introduced in [5]) is that in [19] the quadratic is explored on the whole intersection of the natural box and the trust region, while in [5] only the face determined by an approximate Cauchy point is explored. The subroutine that minimizes the quadratic is called QUACAN and the main algorithm, which handles trust region modifications, is BOX. A comparison between BOX-QUACAN and LANCELOT for box-constrained minimization can be found in [8]. In that paper it was shown that BOX-QUACAN tends to outperform LANCELOT when the objective function is very well approximated by a quadratic. In fact, it seems that the main strength of the algorithm is the way it deals with quadratic subproblems. See [3, 9, 17, 19]. This strength has been fully exploited in engineering problems [10, 11, 12, 14].

The Augmented Lagrangian approach for solving minimization problems with *equality*

constraints and bounds is also well established. According to [6], the complete Augmented Lagrangian algorithm consists of a sequence of outer iterations. At each outer iteration a box-constrained minimization problem is approximately solved whereas Lagrange multipliers and penalty parameters are updated in the master program. BOX-QUACAN is well suited to this scheme. Moreover, if the objective function of the nonlinear program is (almost) quadratic and the equality constraints are (almost) linear, the subproblem solved at each outer iteration is a box-constrained (almost) quadratic problem and, so, we can expect that the overall scheme should be quite efficient. See [10, 11, 12, 13, 14]. An implementation that exploits almost-linearity of the constraints has been given in [25].

Inequality constraints of nonlinear programs can be transformed in equality constraints adding slack variables and bounds. This transformation is quite effective in many cases and allows one to take advantage of the pleasant practical properties of box-constraint solvers in problems that are well approximated by quadratics, when one uses the Augmented Lagrangian approach of [6]. However, it increases the number of variables and, so, it can be inefficient in critical cases. Therefore, it is natural to consider Augmented Lagrangian procedures for dealing with inequality constraints without the slack-variable augmentation. Unfortunately, no Augmented Lagrangian algorithm for inequality constraints (see [2, 24] and references therein) has the property of generating box-constrained quadratic subproblems when applied to quadratic programming with linear inequality constraints. So, it is not clear how efficient an algorithm like BOX-QUACAN would be when used for solving inequality-Augmented Lagrangian subproblems since, no matter how "quadratic" the original problem could be, the subproblems will not be quadratic at all. Moreover, while in the case of equality constraints and bounds the property that "quadratic programs generate quadratic subproblems" strongly suggests the use of the classical Augmented Lagrangian algorithm (which uses the L_2-loss function), the absence of that property in the inequality constrained case opens a large scope of Augmented Lagrangian functions, with probably different numerical properties. In particular, the most classical scheme defines a (piecewise quadratic) Augmented Lagrangian without continuous second derivatives. Other Augmented Lagrangians are two-times differentiable but do not enjoy the property of agreeing with the objective function of the problem within the feasible region.

This paper is organized as follows. In Section 2 we describe the Augmented Lagrangian functions that will be considered in the paper. In Section 3 we introduce the Augmented Lagrangian algorithm and we prove an global convergence result. In Section 4 we explain how BOX-QUACAN is used to solve the subproblems. In Section 5 we show numerical experiments. Conclusions are given in Section 6.

2 Augmented Lagrangian framework

We are concerned with the nonlinear programming problem

$$\text{Minimize } f(x)$$

$$\text{subject to } \quad h(x) = 0, \quad g(x) \leq 0, \quad x \in \Omega,$$

where $f : I\!R^n \to I\!R$, $h : I\!R^n \to I\!R^m$, $g : I\!R^n \to I\!R^p$ are differentiable and Ω is a simple closed and convex set. In general, $\Omega = \{x \in I\!R^n \mid \ell \leq x \leq u\}$. Although all the arguments in this

work apply to the general case, we will restrict ourselves, for simplicity, to the case where no equality constraints are present:

$$\text{Minimize } f(x) \tag{1}$$

$$\text{subject to } \quad g(x) \leq 0, \quad x \in \Omega. \tag{2}$$

The main step of an Augmented Lagrangian method for solving (1-2) is

$$\text{Minimize (approximately) } \; L(x, \rho, \mu) \; \text{ subject to } \; x \in \Omega, \tag{3}$$

where $\rho \in I\!R_{++}$ is a penalty parameter associated to the constraints $g(x) \leq 0$ and $\mu \in I\!R^p_+$ is a vector of Lagrange multiplier estimates.

(Throughout this work, $I\!R_+ = \{t \in I\!R \mid t \geq 0\}$, $I\!R_{++} = \{t \in I\!R \mid t > 0\}$ and $[v]_i$ is the $i-$th component of the vector v.)

The method can also be formulated with p different penalty parameters, one for each component of $g(x)$. The description for this situation is a straightforward variation of the one that we are going to present here. However, it does not seem to have numerical advantages in practical cases.

The objective function of (3) will be called an Augmented Lagrangian if the following properties take place:

P1. For all fixed $\mu \in I\!R^p_+$ (except, perhaps, $\mu = 0$) the method defined by repeated applications of (3) with ρ going to ∞ is a *penalty method* (see [2, 15, 16] among others). This implies that, assuming that the feasible region of (1–2) is nonempty and that x_k is an exact global minimizer of $L(x, \rho_k, \mu)$, every limit point of $\{x_k\}$ is a global solution of (1–2).

P2. If x_* is a regular stationary point of (1–2) and $\mu_* \in I\!R^p_+$ is the vector of Lagrange multipliers then, for all fixed $\rho \in I\!R_{++}$, x_* is a stationary point of

$$\text{Minimize } L(x, \rho, \mu_*) \; \text{ subject to } \; x \in \Omega. \tag{4}$$

An Augmented Lagrangian algorithm consists of repeated applications of (3) followed by the updating of the penalty parameter and the Lagrange multiplier estimates. Generally speaking, the penalty parameter is increased between different iterations if the progress measured in terms of gains of feasibility and complementarity is not satisfactory ($\sum_{i=1}^p [\mu]_i [g(x)]_i$ must be zero at a solution).

The form of *separable* Augmented Lagrangian functions is

$$L(x, \rho, \mu) = f(x) + \sum_{i=1}^{p} R(\rho, \mu_i, g_i(x)). \tag{5}$$

A general way in which suitable Augmented Lagrangian schemes can be obtained (see [2]) is defining

$$R(\rho, \mu_i, g_i(x)) = \frac{1}{\rho} \theta(\rho g_i(x), \mu_i) \tag{6}$$

where $\theta : I\!R \times I\!R_+ \to I\!R$ is a function with the following properties:

$$\lim_{\rho \to \infty} \frac{1}{\rho} \, \theta(\rho z, \mu) = \infty \quad \text{for all} \quad z > 0, \mu > 0 \tag{7}$$

$$\lim_{\rho\to\infty} \frac{1}{\rho}\,\theta(\rho z,\mu) = 0 \quad \text{for all} \quad z<0, \mu>0 \tag{8}$$

$$\frac{\partial}{\partial z}\,\theta(0,\mu) = \mu \quad \text{for all} \quad \mu>0. \tag{9}$$

$$\frac{\partial}{\partial z}\,\theta(z,\mu) \geq 0 \quad \text{for all} \quad z\in I\!R, \mu>0. \tag{10}$$

From now on, if there is no risk of confusion, we write $\theta'(z,\mu) = \frac{\partial}{\partial z}\theta(z,\mu)$. Many variations of this general scheme were introduced and exploited in the literature. In particular, see [4]. Convergence properties of Augmented Lagrangian algorithms for convex problems were recently surveyed in [24]. Due to (7–8), property **P1** holds for Augmented Lagrangians defined by (6). On the other hand, the identity (9) guarantees that property **P2** takes place.

The most classical (Powell-Hestenes-Rockafellar) Augmented Lagrangian method corresponds to

$$\theta_{PHR}(z,\mu) = \frac{(z+\mu)^2}{2} \quad \text{for } z\geq -\mu\ ,\ 0 \ \text{ otherwise.}$$

The main drawback of the PHR Augmented Lagrangian method is that second derivatives of θ_{PHR} are discontinuous, so that methods for solving (3) based on quadratic approximations of the objective function tend to be inefficient.

The exponential-multiplier form of the Augmented Lagrangian (see [1, 2, 27]) overcomes this difficulty defining

$$\theta(z,\mu) = \mu\, e^z \quad \text{for all} \quad \mu>0, z\in I\!R.$$

One of the computational difficulties associated to the exponential penalty function is related to the rapid growth of this function, which can cause overflow and numerical instability.

In fact, the Hessian of the exponential Lagrangian defined above is given by

$$H(x) = \nabla^2 f(x) + \sum_{i=1}^{m} \mu_i e^{\rho g_i(x)} \nabla^2 g_i(x) + \sum_{i=1}^{m} \rho\mu_i e^{\rho g_i(x)} \nabla g_i(x) \nabla g_i(x)^T.$$

The term $\sum_{i=1}^{m} \rho\mu_i e^{\rho g_i(x)} \nabla g_i(x) \nabla g_i(x)^T$ is responsible for the ill-conditioning of $H(x)$ when the coefficients $\rho\mu_i e^{\rho g_i(x)}$ of the rank-one matrices $\nabla g_i(x) \nabla g_i(x)^T$ are large or have very different magnitudes. This is a major reason for controlling the size of these coefficients, which leads one to replace the exponential by a function with a more moderate increasing behavior.

Sometimes stopping by overflow can be avoided without further consequences if the compiler has the capability of replacing the undesirable quantity by the largest possible machine number. This is the case of the problem corresponding to Table 4 of Section 5. In these cases the quantities associated to overflow correspond to trial points that are going to be rejected and the decision on the trust region size taken by BOX is independent of the magnitude of the objective function value at rejected trial points. Therefore, nothing changes if the large quantity is replaced by ∞. However, as we are going to see in other examples, the influence of large quantities on the behavior of the algorithm is more subtle.

Roughly speaking, the level sets of the function $e^{x_1+\ldots+x_n}$ are similar to those of $\max\{x_1,\ldots,x_n\}$ when an x_i is dominant. Moreover, when many components x_i are similar and large the exponential tends to assume a typical "nearly-nonsmooth" shape. In fact,

for any smooth function $f(x_1, \ldots, x_n)$, given a point z where the gradient is not null, the probability of obtaining a point x such that $f(x) < f(z)$ in a neighborhood of radius $\delta > 0$ tends to $\frac{1}{2}$ when $\delta \to 0$. But taking $n = 100$, $z = (100, \ldots, 100)$ and $\delta = 1$ we obtain that the probability of obtaining $e^{x_1+\ldots+x_n} < e^{z_1+\ldots+z_n}$ with $\|x - z\|_\infty < 1$ is around 0.006. On the other hand, the probability of having $\|x\|_2 < \|z\|_2$ with $\|x - z\|_\infty < 1$ is around 0.49 and, of course, the probability of having $\|x\|_\infty < \|z\|_\infty$ with $\|x - z\|_\infty < 1$ is 2^{-100}.

These observations lead us to recommend a modification of the exponential Lagrangian method (suggested in [2]) which consists in replacing the exponential by a quadratic, if the argument exceeds a given parameter, in such a way that the function, the first and second derivatives are continuous.

Therefore, the modification consists in defining

$$\theta(z, \mu) = \mu \, \mathrm{axp}(z),$$

where

$$\mathrm{axp}(z) = e^z \text{ if } z \leq \beta,$$
$$\mathrm{axp}(z) = e^\beta + e^\beta(z - \beta) + e^\beta(z - \beta)^2/2 \text{ if } z > \beta.$$

It is easy to see that Properties **P1** and **P2** hold for this definition.

3 Updating the penalty parameters and the multipliers

Assume that problem (3) has been solved for some $\mu_k \in I\!R^p_+, \rho_k \in I\!R_{++}$ and call x_k the approximate solution obtained. By Property **P2**, if we fixed μ_k and let $\rho_k \to \infty$, the sequence of solutions $\{x_k\}$ would tend to a minimizer of (1-2). This means that, when we solve problem (3) we expect some progress with respect to the previous approximation, both in terms of feasibility and optimality. If this progress is not satisfactory, the penalty parameter should be increased, in general by multiplication by a fixed positive factor γ.

Now, after the resolution of (3) we have enough information to define a new approximation for the vector of Lagrange multipliers. In fact, at a regular solution x_* of (1–2) we have that the property

$$\langle \nabla f(x_*) + \sum_{i=1}^{p} [\mu_*]_i \nabla g_i(x_*), x - x_* \rangle \geq 0 \quad \text{for all} \quad x \in \Omega \tag{11}$$

holds, while at a solution of (3) we have that, approximately,

$$\langle \nabla f(x_k) + \sum_{i=1}^{p} \theta'(\rho g_i(x_k), [\mu_k]_i) \nabla g_i(x_k), x - x_k \rangle \geq 0 \quad \text{for all} \quad x \in \Omega. \tag{12}$$

Comparison between (11) and (12) suggests that a suitable new estimate for the Lagrange multiplier $[\mu_*]_i$ is

$$[\mu_{k+1}]_i = \theta'(\rho g_i(x_k), [\mu_k]_i). \tag{13}$$

(So, according to (10), $\mu_{k+1} \geq 0$.) Therefore, by (12), we have that the property

$$\langle \nabla f(x_k) + \sum_{i=1}^{p} [\mu_{k+1}]_i \nabla g_i(x_k), x - x_k \rangle \geq 0 \quad \text{for all} \quad x \in \Omega \tag{14}$$

is satisfied, approximately, after each outer iteration of an Augmented Lagrangian method.

In the nonlinear programming terminology, formula (13) defines a first-order multiplier update. It represents just one of the ways of predicting the correct multipliers at the solution, but not the most accurate one. In fact, higher order multiplier predictions can be defined (see [2, 16]) but they usually require additional costly calculations. Except for small-scale problems, we prefer the estimate (13) which, on the other hand, can be interpreted (for convex problems) in terms of the proximal point algorithm on the dual space (see [24] and references therein).

Assume, for a moment, that (14) holds up to a user-given small precision $\varepsilon > 0$. If, in addition, we have that

$$g_i(x_k) \leq \varepsilon \quad \text{for all} \quad i = 1, \ldots, p \tag{15}$$

and

$$[\mu_{k+1}]_i \leq \varepsilon \quad \text{whenever} \quad g_i(x_k) < -\varepsilon \tag{16}$$

we say that x_{k+1} is an approximate solution of the original problem. (In fact, it is an approximate stationary point of (1–2).)

In order that, eventually, approximate stationary points can be reached, we require that the precision $\varepsilon_k > 0$ that define (3) must be such that $\varepsilon_k = \varepsilon$ after a finite number of iterations.

Taking into account the observations above, a practical Augmented Lagrangian algorithm can be defined by:

Augmented Lagrangian algorithm

Step 1 *Initialization*

Choose $\tau \in (0,1), \gamma > 1,\ \rho_1 > 0,\ [\mu_1]_i > 0 \quad \text{for all} \quad i = 1, \ldots, p,\ \varepsilon_1 > 0,\ \sigma_0 = 0$. Set $k \leftarrow 1$.

Step 2 *Solve the subproblem*

Solve (3) up to precision ε_k.

Step 3 *Update Lagrange multipliers*

Compute μ_{k+1} according to (13).

Step 4 *Stopping criterion*

If $\varepsilon_k = \varepsilon$ and, in addition, (15) and (16) hold, declare "convergence" and terminate the execution of the algorithm.

Step 5 *Update penalty parameter and precision*

Define ε_{k+1} and

$$\sigma_k = \max \{|\ \min \{[\mu_k]_i, -g_i(x_k)\}|,\ i = 1, \ldots, p\}.$$

If $\sigma_k \leq \tau \sigma_{k-1}$, define $\rho_{k+1} = \rho_k$. Else, define $\rho_{k+1} = \gamma \rho_k$.

Step 6 *Increase iteration number*

Replace k by $k+1$ and go to **Step 2.**

Let us finish this section giving an global convergence result for the Augmented Lagrangian algorithm defined above. First, we need to specify the meaning of Step 2. Define, for all $x \in \Omega, \rho > 0, \mu \in I\!R^p_+$,

$$G(x, \rho, \mu) = P(x - [\nabla f(x) + \sum_{i=1}^{p} \theta'(\rho g_i(x), \mu) \nabla g_i(x)]) - x,$$

where $P(z)$ is the projection of z on Ω. In terms of the function G, the stopping criterion defined by Step 2 will be

$$\|G(x, \rho, \mu)\| \leq \varepsilon_k, \tag{17}$$

where $\|\cdot\|$ is an arbitrary norm.

In order to analyze the global behavior of the algorithm, we set $\varepsilon = 0$ and we replace the requirement that $\varepsilon_k = \varepsilon$ after a finite number of iterations by $\varepsilon_k \to 0$.

We will need two additional assumptions on θ. These assumptions are clearly satisfied by the specific Augmented Lagrangians in which we are interested:

$$\lim_{z \to \infty} \frac{\partial}{\partial z} \theta(z, \mu) = \infty \tag{18}$$

and

$$\lim_{z \to -\infty} \frac{\partial}{\partial z} \theta(z, \mu) = 0. \tag{19}$$

A stationary point of (1-2) is a point $x_* \in \Omega$ such that there exists $\mu_* \in I\!R^p_+$ satisfying

$$\langle \nabla f(x_*) + \sum_{i=1}^{p} [\mu_*]_i \nabla g_i(x_*), x - x_* \rangle \geq 0 \quad \text{for all} \quad x \in \Omega, \tag{20}$$

$$g(x_*) \leq 0 \tag{21}$$

and

$$[\mu_*]_i g_i(x_*) = 0, \ i = 1, \ldots, p. \tag{22}$$

As it is well known (see [16, 20]), under suitable constraint qualifications, minimizers of (1-2) must be stationary points in the sense of (20-22).

Theorem 2.1. *Assume that Ω is compact and that $\{\mu_k\}$ is bounded. Then, every limit point of $\{x_k\}$ is stationary for (1-2).*

Proof. Let K_1 be an infinite subset of indices such that $\{x_k\}_{k \in K_1}$ is convergent and take an appropriate subset $K_2 \subset K_1$ such that $\{\mu_{k+1}\}_{k \in K_2}$ is convergent too. Thus, $\lim_{k \in K_2} x_k = x_*$ and $\lim_{k \in K_2} \mu_{k+1} = \mu_*$. By (17) we have that

$$\|G(x_k, \rho_k, \mu_k)\| \leq \varepsilon_k.$$

Therefore, by (13),

$$\|P(x_k - [\nabla f(x_k) + \sum_{i=1}^{p} [\mu_{k+1}]_i \nabla g_i(x_k)]) - x_k\| \leq \varepsilon_k$$

and, taking limits for $k \in K_2$,

$$\|P(x_* - [\nabla f(x_*) + \sum_{i=1}^{p} [\mu_*]_i \nabla g_i(x_*)]) - x_*\| = 0.$$

By the convexity of Ω, this implies that (20) holds.

Now, we consider two cases. In the first case there exists $k_0 \in \mathbb{N}$ such that $\sigma_{k+1} \leq \tau\sigma_k$ for all $k \geq k_0$. Therefore, $\sigma_k \to 0$ which, by continuity, implies that

$$\min \{[\mu_*]_i, -g_i(x_*)\} = 0, \quad i = 1, \ldots, p.$$

Therefore, (21) and (22) hold.

In the second case, $\rho_k \to \infty$. By (18) and the boundedness of $\{\mu_k\}$, the fact that $\theta'(\rho_k g_i(x_k), [\mu_k]_i)$ is bounded implies that $\rho_k g_i(x^k)$ admits an upper bound. But, since $\rho_k \to \infty$, this implies that $\limsup g_i(x_k) \leq 0$. Therefore, by continuity, $g_i(x_*) \leq 0$ for all $i = 1, \ldots, p$. So, (21) holds.

Now, suppose that $g_i(x_*) < 0$. For $k \in K_2$ large enough we have that

$$g_i(x_k) \leq g_i(x_*)/2 < 0,$$

so

$$\lim_{k \to \infty} \rho_k g_i(x_k) = -\infty.$$

By (19) and the boundedness of μ_k this implies that

$$\lim_{k \to \infty} \theta'(\rho_k g_i(x_k), [\mu_k]_i) = 0.$$

So, $[\mu_{k+1}]_i \to 0$ and, consequently, $[\mu_*]_i = 0$. This means that the complementarity condition (22) also holds. This completes the proof.

It must be warned that the hypothesis on the boundedness of $\{\mu_k\}$ is strong and that it might not hold in critical situations. For example, a problem could not contain stationary points in the sense of (20-22) but could have a non-regular global minimizer. If we apply the algorithm to a problem like that, the multipliers will not be bounded. In fact, by Theorem 2.1, boundedness of $\{\mu_k\}$ would imply existence of stationary points. Nevertheless, very likely, the algorithm will converge to the non-regular global minimizer.

If x_k is close to a regular solution of (1-2) and μ_k is close to the corresponding vector of Lagrange multipliers, we expect that approximately solving the Augmented Lagrangian subproblem would represent an effective progress towards the solution, at least if the penalty parameter is sufficiently large. In this case, the test $\sigma_{j+1} \leq \tau\sigma_j$ tends to hold for all $j \geq k$ and the penalty parameter remains bounded, thus providing numerical stability.

4 Solving the subproblems

Assume that Ω is an n-dimensional box, given by

$$\Omega = \{x \in \mathbb{R}^n \mid \ell \leq x \leq u\}.$$

So, (3) consists in finding an approximate solution of

$$\text{Minimize}_x \;\; L(x, \rho, \mu) \text{ subject to } \ell \leq x \leq u. \tag{23}$$

Augmented Lagrangian algorithms with approximate solutions of the subproblems were analyzed in [6, 10, 22, 23].

Subproblem (23) is solved, at each outer iteration, using BOX-QUACAN [19]. As it was mentioned in the Introduction, BOX-QUACAN is an algorithm that minimizes functions with bounds on the variables by means of sequential (approximate) minimization of second-order quadratic approximations with simple bounds. The bounds for the quadratic model come from the intersection of the original box with a trust region defined by the $\infty-$norm. The Augmented Lagrangian algorithm is designed in order to cope with large-scale problems. For this reason, no factorization of matrices are used at any stage. The quadratic solver used to deal with the subproblems of the box-constrained algorithm visits the different faces of its domain using conjugate gradients on the interior of each face and "chopped gradients" as search directions to leave the faces. See [17], [19] and [3] for a description of the 1998 implementation of QUACAN. At each iteration of this quadratic solver, a matrix-vector product of the Hessian approximation and a vector is needed. Since Hessian approximations are usually cumbersome to compute, we use the "Truncated Newton" approach, so that each *Hessian* $\times$ *vector* product is replaced by an incremental quotient of ∇L along the direction given by the vector.

The Augmented Lagrangian subroutine has many parameters that influence its practical performance. In this study we adjusted the most sensitive parameters using a typical problem with 103 variables and 78 nonlinear constraints, called "the Icosahedron problem". (This is problem 1 (3, 12) described below, with the inequality constraints replaced by equality constraints by means of the introduction of slack variables.) Below we comment the decision taken on the main sensitive parameters based on this problem.

4.1 Termination criteria for the box-constraint solver

Each outer iteration finishes when some stopping criterion for the algorithm that solves (23) is fulfilled. We consider that the box-constraint algorithm converges when

$$\|g_P(x)\|_2 \leq \varepsilon_k,$$

where $g_P(x)$ is the "continuous projected gradient" of the objective function of (23) at the point x. This vector is defined as the difference between the projection of $x - \nabla L(x, \rho, \mu)$ on the box and the point x. The tolerance ε_k may change at each outer iteration. In fact, we tested (with the Icosahedron problem) a strategy that defines dynamically ε_k depending on the degree of feasibility of the current iterate against a constant choice $\varepsilon = 10^{-5}$. Although not conclusive, the results for constant ε in the typical problem were better. So, we adopted this choice in the experiments. The box-constraint code admits other stopping criteria. For example, the execution also stops when the radius of the trust region becomes too small (less than 10^{-8} in our experiments) or when the number of iterations exceeds a user-given value (300 in our experiments).

4.2 Parameters for the Quadratic Solver

The algorithm QUACAN, which minimizes a (not necessarily convex) quadratic with bounds on the variables, plays a crucial role in the overall behavior of the Augmented Lagrangian method. Therefore, its main parameters must be carefully chosen. A very important one is the parameter used to declare convergence of the algorithm. If the projected gradient of the quadratic is null, the corresponding point is stationary. According to this, convergence is declared if the norm of this projected gradient is less than a fraction of the corresponding norm at the initial point. Here we use "non-continuous projected gradients", in which the projections are not computed on the feasible box but on the affine subspace defined by the active constraints. After testing the fractions 1/10, 1/100 and 1/100000 on the Icosahedron Problem, we observed that the first was the best one, so it was the one employed in the numerical experiments. The number of iterations allowed to the quadratic solver is also important because, sometimes, a lot of effort is invested in solving subproblems without a close relation to the original problem. We found that 100 is a suitable value for "maximum of iterations" in this case. Other non-convergence stopping criteria were inhibited in the resolution of the quadratic subproblem.

The radius of the trust region determines the size of the domain of the auxiliary box used in QUACAN. The nonlinear programming algorithm is sensitive to the choice of δ, the first trust region radius. In the experiments presented in this paper we used $\delta = 10$.

A very important parameter of the quadratic solver is $\eta \in (0, 1)$. According to this parameter, it is decided whether the next iterate must belong or not to the current face. Roughly speaking, if η is small the algorithm tends to leave the current face when a mild decrease of the quadratic is detected. On the other hand, if $\eta \approx 1$, the algorithm only abandons the current face when the current point is close to a stationary point of the quadratic on that face. A rather surprising result was that the conservative value $\eta = 0.95$ was better than smaller values of η for the Icosahedron Problem.

When the quadratic solver hits the boundary of its feasible region an extrapolation step can be tried, according to the value of an extrapolation parameter $\kappa \geq 1$. If κ is large new points will be tried at which the number of active constraints can be considerably increased. On the other hand, if $\kappa = 1$, no extrapolation is intended. Here, we finished up deciding that $\kappa = 10$ is suitable for the Icosahedron Problem.

4.3 Convergence results of BOX and QUACAN

The box-constraint solver BOX is a trust region method. Its general convergence results have been given in [19]. Roughly speaking, if the objective function has continuous partial derivatives and the Hessian approximations are bounded, every limit point of a sequence generated by BOX is stationary. When one uses true Hessians or secant approximations (see [7]) and the quadratic subproblems are solved with increasing accuracy, superlinear or quadratic convergence can be expected. In our implementation, we used a fixed tolerance as stopping criterion for the quadratic solver QUACAN, because the benefits of high-order convergence of BOX would not compensate increasing the work of the quadratic solver.

According to the numerical results in [8, 10, 11, 12, 13] and our own experience, the main reason for the efficiency of BOX is the strategy used by the quadratic solver QUACAN for han-

dling active constraints. The first version of QUACAN was given in [17] for (not necessarily strictly) convex quadratics. In the method introduced in [17] successive consecutive iterates within a particular face of the domain are generated using conjugate gradients. However, this generation is interrupted when the iterate becomes infeasible or when it is "approximately stationary" in the current face. In the first case, projections are used for computing a new point in a different face where, possibly, many active constraints are added. This strategy is different from the one used in [26] (called "truncated Newton" in [17]), where infeasible conjugate gradient iterates are admitted in the affine subspace that contains the current face until an approximate Newton direction is obtained. It has been pointed out in [17] that in the presence of almost-singular Hessians the effort of computing almost-Newton directions is not worthwhile. Moreover, if the feasible region is "small" (as occurs in the trust region context) and/or the unconstrained minimizer of the quadratic is very infeasible, the quadratic behaves as a linear function within the feasible box and gaining active constraints as soon as possible tends to increase efficiency of the overall algorithm.

In [17] an iterate is declared "approximately stationary" in the current face when it can be guaranteed that the functional value at a new computable iterate outside the face is less than the minimum of the quadratic in an internal ball centered in the current iterate. The new iterate is computed along the "chopped-gradient" direction, for which a physical interpretation was given in [9]. As a result of this property, the quadratic solver finds a solution of the problem in a finite number of iterations, independently of possible singularity of the Hessian and even when dual-degenerate points exist.

Further versions of QUACAN were described in [3, 18, 19]. In [3, 18] alternative directions to conjugate gradients are considered within the faces. However, conjugate gradients are still used in the version of QUACAN used in the present research. More important is the fact that in [3, 19] QUACAN was extended in order to handle nonconvex problems. In this case, it can be proved that convergence occurs in the sense that there exists a limit point of the generated sequence which must be stationary, but not necessarily a global minimizer. However, if dual-degenerate points do not exist, all the iterates belong, eventually, to the same face and, as a consequence, finite convergence to a stationary point of the quadratic problem occurs.

5 Numerical experiments

We tested the classical PHR Augmented Lagrangian method and the modified exponential Lagrangian method using some typical nonlinear programming problems. In our experiments we used $\tau = 0.1, \gamma = 10$, $\rho_1 = 10$, $[\mu_1]_i = 1$ for the exponential Lagrangian method and $[\mu_1]_i = 0$ for PHR.

Problem 1: Find *npun* points on the unitary sphere of $I\!R^{ndim}$ such that maximum scalar products between them is minimum. (This is equivalent to say that the minimum distance is maximum.) The nonlinear programming problem has been defined as

$$\text{Minimize } z$$

$$\text{subject to}$$

$$\|x_k\|_2^2 = 1, k = 1, \ldots npun,$$

$$z \geq \langle x_i, x_j \rangle \text{ for all } i \neq j.$$

$$x_k \in I\!R^{ndim}, k = 1, \ldots, npun.$$

The solution of this problem for $ndim = 3, npun = 24$ is the set of vertices of the polyhedron showed in Picture 1.

As initial approximation we took $[x_k]_i$ and z randomly in $[-1, 1]$. In Tables 1, 2 and 3 we show the performance of the Augmented Lagrangian PHR method and the modified exponential Lagrangian method for $(ndim, npun) = (3, 24), (3, 30)$ and $(4, 25)$ respectively and for different choices of β. The configuration of the tables for all the problems is similar:

"Outer" is the number of Augmented Lagrangian iterations (number of times in which (3) is solved;

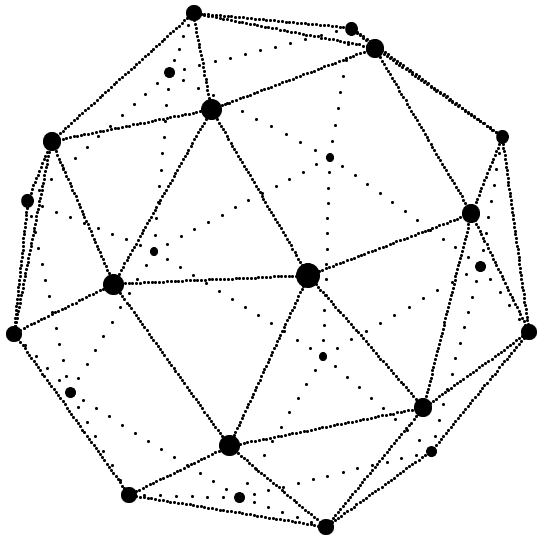
"Inner" is the number of iterations performed by BOX;

"Evaluations" is the number of times in which the Augmented Lagrangian was evaluated;

"Q.It." is the number of iterations of QUACAN;

"MVP" is the number of "matrix vector products", which in this case involve an additional Augmented Lagrangian gradient evaluation;

"Time" is the CPU time (seconds) of the execution using Microsoft double precision Fortran 77 in a Pentium with 90 MHz.



Picture 1: Solution of Problem 1 (3, 24)

For this problem, the last column "dist" is the minimum distance between points at the solution obtained. (In fact, to prevent small violations of equality constraints, the solution computed by the algorithm was first normalized so that all the points "really" belong to

the unitary sphere.) This problem has *npun* equality constraints. Since for this class of constraints the classical PHR Augmented Lagrangian scheme does not present discontinuity problems, we dealt with such constraints using the standard procedure.

Problem 2: The objective is to draw a map of America in which the countries appear with areas that are proportional to their real values. The unknowns are 132 points in $\mathbb{R}^2$, which define the boundaries of 17 countries. Each point is assigned to the boundary of one or more countries. The computed area of each country is calculated as a function if its boundary points using Green's formula. The constraints of the problem are:

$$0.99 \times \text{True area} \leq \text{Computed area} \leq 1.01 \times \text{True area}$$

for each country. As initial approximation we took the coordinates of the 132 points in the New York Times map of America which, of course, do not fit with true areas. The objective function is $\frac{1}{2}\sum_{j=1}^{132} \|P_j - Q_j\|_2^2$, where $P_1, \ldots, P_{132}$ are the unknowns and $Q_1, \ldots, Q_{132}$ is the initial approximation. The solution of this problem is the map of America drawn in Picture 2.

Problem 3: This problem has been suggested by C. Gonzaga [21] to test sensitivity with respect to almost coincident constraints. It is a very simple problem which, on purpose, is not formulated in the best possible way. (Bound constraints are treated as explicit constraints $g_i(x) \leq 0$ instead of being included in Ω.) The problem is

$$\text{Minimize } \sum_{i=1}^{n} \frac{[x]_i}{i} \text{ subject to } [x]_i \geq 0,\ [x]_i \geq 0.001, i = 1, \ldots, n.$$

Clearly, its solution is $(0.001, \ldots, 0.001)$. We used $n = 1000$ (so $p = 2000$). The coordinates of the initial approximation were taken randomly between -10 and 10. The last column in Table 5 is the logarithm of the $\infty-$norm of the error.

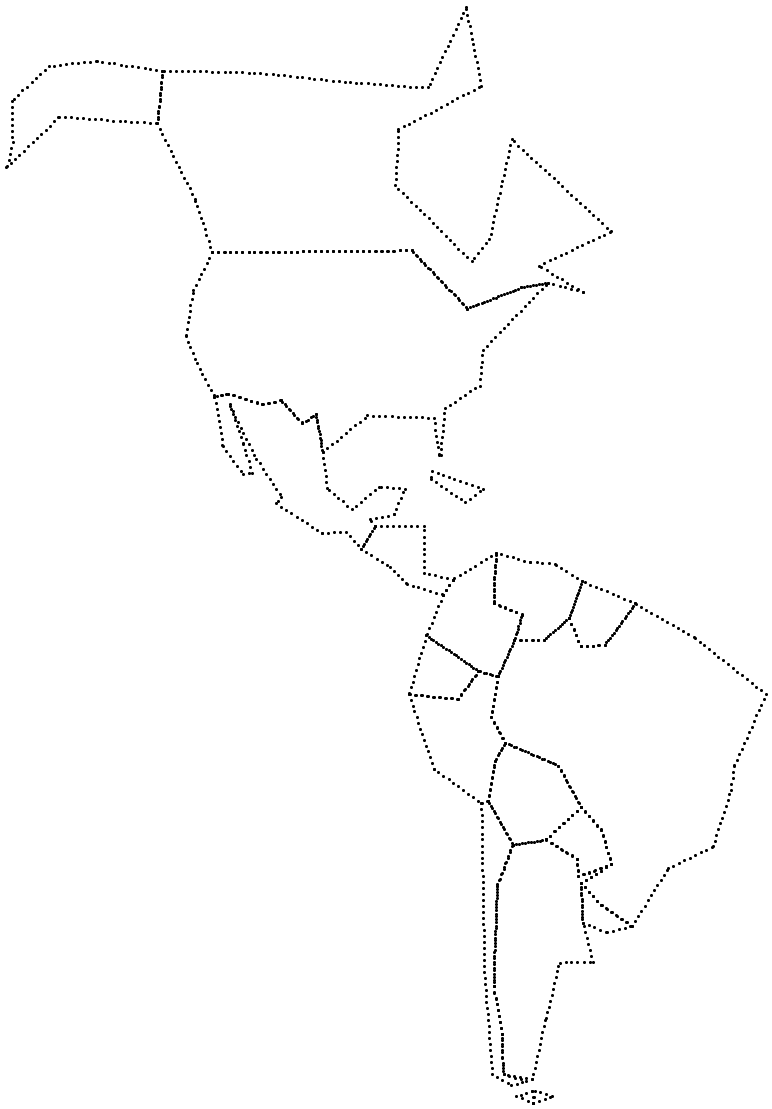
Problem 4: This problem consists in finding *npun* points in $\mathbb{R}^3$ such that the distance between any pair of them is not less than 1 and the maximum distance is as close to 1 as possible:

$$\text{Minimize } z$$

$$\text{subject to}$$

$$1 \leq \|x_i - x_j\|_2^2 \leq 1 + z$$

for all $i \neq j$, $i, j = 1, \ldots, npun$. The coordinates of the initial approximation were taken randomly between -10 and 10. After solving the problem using the Augmented Lagrangian method, we computed the effective distances $\|x_i - x_j\|$. If any of them is (of course, slightly) smaller than 1, we replaced each x_k by a factor times x_k" in such a way that the smallest distance is exactly equal to 1. For this normalized points we computed the maximum deviation of the distances with respect to 1. This number is the one on the last column of Tables 6 and 7 and reflects the quality of the solution obtained in practice.



Picture 2: Solution of Problem 2

Table 1: Problem 1 (3, 24) (n = 72, m = 24, p = 276)

Method	Outer	Inner	Evaluations	Q.It.	MVP	Time	dist
PHR	7	503	5069	15742	43976	316.0	.743830
$\beta = 0.$	6	48	78	1115	1396	69.5	.744206
$\beta = 0.1$	5	51	78	1125	1419	70.7	.744206
$\beta = 1.$	5	55	85	1336	1703	84.6	.744206
$\beta \geq 10$	5	61	94	1453	1843	92.0	.744206

Table 2: Problem 1 (3, 30) (n = 90, m = 30, p = 435)

Method	Outer	Inner	Evaluations	Q.It.	MVP	Time	dist
PHR	8	434	3945	26990	47418	420.8	.657374
$\beta = 0.$	5	125	193	6057	6995	489.8	.660981
$\beta = 0.1$	5	124	187	5558	6446	456.9	.660981
$\beta = 1.$	5	138	216	5999	6770	479.0	.660981
$\beta = 10.$	5	160	242	6621	7593	532.9	.660981
$\beta = 20.$	5	157	233	6206	7202	507.0	.660981
$\beta = 100.$	5	157	233	6206	7202	507.0	.660981

Table 3: Problem 1 (4, 25) (n = 100, m = 25, p = 600)

Method	Outer	Inner	Evaluations	Q.It.	MVP	Time	dist
PHR	7	635	4726	34528	64374	658.4	.957825
$\beta = 0.$	9	2451	5406	132620	156111	8927.8	.787241
$\beta = 0.1$	10	2762	6496	107417	128496	7416.5	.663185
$\beta = 1.$	6	202	314	14404	15561	952.5	.961487
$\beta = 10.$	6	237	380	15609	17192	1067.5	.961489
$\beta = 20.$	6	258	398	15772	17291	1074.0	.961487
$\beta = 100.$	6	258	398	15772	17291	1073.6	.961487
$\beta = 500.$	6	258	398	15772	17291	1073.5	.961487

Table 4: Problem 2 (n = 264 , p = 34)

Method	Outer	Inner	Evaluations	Q.It.	MVP	Time	f
PHR	7	110	931	3508	8505	162.4	3.050771
$\beta = 0.$	6	56	87	1493	2083	79.9	3.049630
$\beta = 0.1$	6	57	88	1367	1910	74.3	3.049630
$\beta = 1.$	6	64	98	1485	2183	85.1	3.049630
$\beta = 10.$	6	72	109	1287	1880	74.0	3.049630
$\beta = 20.$	6	80	115	1227	1717	68.5	3.049630
$\beta \in [100., 696.]$	6	109	139	973	1451	59.0	3.049630
$\beta \geq 697.$							overflow

Table 5: Problem 3 (n = 1000 , p = 2000)

Method	Outer	Inner	Evaluations	Q.It.	MVP	Time	log(Error)
PHR	6	331	964	9193	21446	1333.0	0.83
$\beta = 0.$	6	94	139	9578	13087	1400.1	-8
$\beta = 0.1$	6	104	158	10935	14969	1609.2	-8
$\beta = 1.$	6	113	171	11523	16329	1736.9	-8
$\beta = 10.$	6	136	198	10430	15071	1634.8	-8
$\beta = 20.$	6	149	217	11318	16325	1754.4	-8
$\beta = 100.$	6	224	287	12236	17646	1899.8	-8

Table 6: Problem 4 (3, 10) (n = 31 , p = 90)

Method	Outer	Inner	Evaluations	Q.It.	MVP	Time	deviation
PHR	9	143	369	1910	4070	19.7	.776874
$\beta = 0.$	3	48	70	565	722	31.4	.773190
$\beta = 0.1$	3	52	79	692	905	38.9	.773183
$\beta = 1.$	2	45	68	500	683	29.8	.762397
$\beta = 10.$	3	67	96	743	961	41.9	.773175
$\beta = 20.$	3	132	195	1741	2151	92.4	.803061
$\beta = 100.$	3	161	248	994	1459	65.6	.773175

Table 7: Problem 4 (3, 20) (n = 61 , p = 380)

Method	Outer	Inner	Evaluations	Q.It.	MVP	Time	deviation
PHR	6	314	844	5035	11532	120.1	1.537385
$\beta = 0.$	4	75	112	2020	2409	711.1	1.446678
$\beta = 0.1$	4	63	89	1498	1733	512.7	1.446662
$\beta = 1.$	4	95	138	2416	2875	857.4	1.446650
$\beta = 10.$	4	88	132	2399	2725	811.3	1.446650
$\beta = 20.$	4	108	161	2161	2598	781.6	1.446650
$\beta = 100.$	4	175	268	2249	2718	839.0	1.446650

6 Conclusions

A qualitative analysis of the numerical results presented in Tables 1–8 shows that:

1. The exponential Lagrangian method with $\beta = 0$ is the best method in Problem 1 (3,24). The difference with $\beta = 0.1$ is, however, marginal. The performance of PHR is much poorer in this problem.

2. In Problem 1 (3,30) the best performance is the one of the exponential Lagrangian method with $\beta = 0.1$. PHR uses less computer time but the quality of the solution is worse. In spite of using less computer time, the number of matrix-vector products and the other quantitative indicators is much larger for PHR than for exponential Lagrangian methods. This phenomenon is partially due to the higher cost of exponentials with respect to quadratics. However, more influent in the computer time is the fact that, for PHR, it is not necessary to evaluate the gradient of a constraint at a point where it is strongly satisfied, whereas for exponential Lagrangian algorithms all the constraint gradients must be evaluated independently of their degree of fulfillment.

3. In Problem 1 (4, 25), the exponential Lagrangian method with $\beta = 1$ is the best one. PHR uses less computer time, but the solution is worse and the number of MVP is four times larger than the winner one. In this case $\beta = 0$ and $\beta = 0.1$ give low-quality solutions while the solution for $\beta > 1$ has the same quality as that of $\beta = 1$.

4. In Problem 2, the solution has the same quality for all the exponential Lagrangian methods but is marginally worse for PHR. In this problem the computer time decreases as β increases, but the number of inner iterations goes in the opposite direction. This means that, when β grows, the quadratic subproblems become easier and less MVP are necessary to achieve the required precision by QUACAN. As a result, more BOX iterations are necessary, but savings on MVP turn these alternatives more economic.

5. The most remarkable fact in Problem 3 is the poor quality of the solution obtained by PHR. All the exponential Lagrangian methods behaved similarly, with some advantage for $\beta = 0$. In fact, although the exponential Lagrangian methods were able to find the solution, their behavior in terms of quantitative indicators was far from being satisfactory. Although this problem has been introduced with the aim of testing the influence of almost coincident constraints ($[x]_i \geq 0$ and $[x]_i \geq 0.001$) additional

experiments using only $[x]_i \geq 0$ gave similar results. The key point seems to be the large number of active constraints at the solution, combined with the very different influence of the variables on the variation of the objective function. Both features make quadratic models inadequate. On the other hand, if the problem is scaled so that the variable $[x]_i$ is replaced by $[x]_i/i$ all the algorithms behave very well. Moreover, the algorithms (especially PHR) also behave very well if the initial approximation belongs to $[-20, -10]^n$ because in this case all the inner iterates tend to lie in a region that is infeasible with respect to all the constraints, where there exists a well conditioned quadratic model that represents well the true objective function of the subproblems. Recall that other obvious situation in which the problem is trivial is when the bounds are included in Ω, so that QUACAN deals with them. As a matter of fact, it seems that the minimization of $\sum_{i=1}^{1000} [x]_i/i$ subject to $x \geq 0$ is a very simple and surprisingly challenging problem for testing Augmented Lagrangian methods.

6. In Problem 4 (3,10) the best solution is obtained by the exponential Lagrangian method with $\beta = 1$, which also uses the lowest computer time among exponential Lagrangians. PHR uses less computer time (although more MVP) but the quality of its solution is marginally worse.

7. Finally, in Problem 4 (3,20) PHR is the method that uses less computer time, but its solution is worse than all the solutions obtained by exponential Lagrangians. Among these, $\beta = 1$ is the best in terms of computer time, its solution being very marginally worse than that of $\beta > 1$.

Summing up, it appears from the numerical experiments that the solutions obtained by PHR are, in general, worse than those obtained by the exponential Lagrangian algorithm. This deficiency is related to lack of continuity in second derivatives. In fact, when second derivatives change abruptly, the model approximation ceases to be of second-order, fast convergence rate is lost and BOX tends to stop with diagnostics of "small trust region", instead of "small projected gradient". The consequence is that a really small projected gradient and thus a good solution sometimes fails to be reached.

The expensiveness of exponential Lagrangian inner iterations and matrix-vector products with respect to the same indicators of PHR is also very impressive. As we mentioned above, the main reason is that one MVP in the case of the exponential Lagrangian involves necessarily all the constraints, while in PHR it involves only those which are not strongly satisfied.

The experiments presented in the previous section also reveal that the quadratic modification of the exponential Lagrangian method has advantages over the original algorithm. Although we cannot determine accurately the best possible value for β, it seems that for reasonably scaled problems some value around the unity is the best one.

In the next table, we show the number of matrix-vector products (so, auxiliary gradient evaluations) per inner iteration for the best choice of β at each problem. We also show the ratio between this number and the number of variables.

Table 8: Gradient evaluations

Table	MVP	Inner	MVP/Inner	MVP/Inner/n
1	1396	48	29	0.40
2	6995	25	56	0.62
3	15561	202	77	0.77
4	1451	109	13	0.05
5	13087	94	139	0.14
6	683	45	15	0.48
7	1733	63	28	0.46

This table shows that a considerable number of gradient evaluations per iteration is used in the truncated Newton approach for all the problems, except for the problem of Table 4, in which this number is very moderate. In one case (Table 3) the number of gradient evaluations per iteration is 77 percent of the number that would be used by a discrete Newton method.

The observation above shows that there is a lot of place for the development of quasi-Newton methods for problems with the described structure since, essentially these methods use only one gradient evaluation per iteration. Of course, we do not expect to reproduce the number of inner iterations of a truncated Newton method using quasi-Newton but it seems that even losing in terms of number of iterations, a quasi-Newton method could be more efficient in terms of overall performance. A little bit disappointing is the fact that we have tested the use of classical BFGS and Symmetric Rank-One corrections for these problems with results much poorer than the ones of the truncated Newton method.

A final observation related to the practical objectives formulated in the Introduction of this paper comes from observing the behavior of the Augmented Lagrangian Algorithms in Problem 3. It seems that there is a considerable price to be paid for using "quadratic-intensive" algorithms for solving non-quadratic iterative reformulations of quadratic problems. Therefore, the slack-variable transformation continues being an interesting alternative if the ratio between number of constraints and number of variables is not very large.

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References

[1] R. R. Allran and S. E. V. Johnsen [1970], An algorithm for solving nonlinear programming problems subject to nonlinear inequality constraints, *Computer Journal* 13, pp. 171-177.

[2] D. P. Bertsekas [1982], *Constrained optimization and Lagrange multiplier methods*, Academic Press, New York.

[3] R. H. Bielschowsky, A. Friedlander, F. M. Gomes, J. M. Martínez and M. Raydan [1998], An adaptive algorithm for bound constrained quadratic minimization, *Investigación Operativa* 7, pp. 67-102.

[4] R. A. Castillo [1998], *Métodos de Lagrangeano aumentado usando penalidades generalizadas para programação não linear*, Tese de Doutorado, COPPE, Universidade Federal do Rio de Janeiro.

[5] A. R. Conn, N. I. M. Gould and Ph. L. Toint [1988], Global convergence of a class of trust region algorithms for optimization with simple bounds, *SIAM Journal on Numerical Analysis* 25, pp. 433 - 460. See also *SIAM Journal on Numerical Analysis* 26 (1989) pp. 764 - 767.

[6] A. R. Conn, N. I. M. Gould and Ph. L. Toint [1991], A globally convergent Augmented Lagrangean algorithm for optimization with general constraints and simple bounds, *SIAM Journal on Numerical Analysis* 28, pp. 545 - 572.

[7] J. E. Dennis and R. B. Schnabel [1983], *Numerical methods for unconstrained optimization and nonlinear equations*, Prentice-Hall, Englewood Cliffs, N. J.

[8] M. A. Diniz-Ehrhardt, M. A. Gomes-Ruggiero and S. A. Santos [1997], Comparing the numerical performance of two trust region algorithms for large-scale bound-constrained minimization, *Investigación Operativa* 7, pp.23-54.

[9] Z. Dostál [1997], Box constrained quadratic programming with proportioning and projections, *SIAM Journal on Optimization* 7, pp. 871–887.

[10] Z. Dostál, A. Friedlander and S. A. Santos [1998], Solution of coercive and semicoercive contact problems by FETI domain decomposition, *Contemporary Mathematics* 218, pp. 82–93.

[11] Z. Dostál, A. Friedlander and S. A. Santos [1997], Solution of contact problems using subroutine BOX-QUACAN, *Investigación Operativa* 7, pp.13-22.

[12] Z. Dostál, A. Friedlander and S. A. Santos [1997], Analysis of block structures by Augmented Lagrangians with adaptive precision control, *Proceedings of GEOMECHANICS'96*, ed. Z. Rakowski, A. A. Balkema, Rotterdam, pp.175-180.

[13] Z. Dostál, A. Friedlander and S. A. Santos [1997], Augmented Lagrangians with Adaptive Precision Control for Quadratic Programming with Equality Constraints, to appear in *Computational Optimization and Applications.*

[14] Z. Dostál, A. Friedlander, S. A. Santos and I. Malík [1997], Analysis of semicoercive contact problems using symmetric BEM and Augmented Lagrangians, *Engineering Analysis with Boundary Elements* 18, pp.195-201.

[15] A. V. Fiacco and G. P. Mc Cormick [1968], *Nonlinear programming: sequential unconstrained minimization techniques*, John Wiley, New York.

[16] R. Fletcher [1987]: *Practical Methods for Optimization*, John Wiley and Sons, Chichester.

[17] A. Friedlander and J. M. Martínez [1994], On the maximization of a concave quadratic function with box constraints, *SIAM Journal on Optimization* 4, pp. 177-192.

[18] A. Friedlander, J. M. Martínez and M. Raydan [1995], A new method for large-scale box constrained convex quadratic minimization problems, *Optimization Methods and Software* 5 pp. 57-74.

[19] A. Friedlander, J. M. Martínez and S. A. Santos [1994], A new trust region algorithm for bound constrained minimization, *Applied Mathematics and Optimization* 30, pp. 235-266.

[20] P. E. Gill; W. Murray; M. H. Wright [1981], *Practical optimization*, Academic Press, London.

[21] C. C. Gonzaga [1997], Private communication.

[22] W. W. Hager [1985], Approximations to the multiplier method, *SIAM Journal on Numerical Analysis* 22, pp. 16–46.

[23] W. W. Hager [1987], Dual techniques for constraint optimization, *Journal of Optimization Theory and Applications* 55, pp. 37–71.

[24] A. N. Iusem [1999], Augmented Lagrangian and proximal point methods for convex optimization, *Investigación Operativa* 8, pp. 11-50.

[25] N. Krejić, J. M. Martínez, M. P. Mello and E. A. Pilotta [2000], Validation of an Augmented Lagrangian algorithm with a Gauss-Newton Hessian approximation using a set of hard-spheres problems, *Computational Optimization and Applications* 16, pp. 247-263.

[26] J. J. Moré and G. Toraldo [1991], On the solution of large quadratic programming problems with bound constraints, *SIAM Journal on Optimization* 1, pp. 93-113.

[27] F. H. Murphy [1974], A class of exponential penalty functions, *SIAM Journal on Control* 12, pp. 679-687.