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RAIRO. Recherche opérationnelle, tome 26, n° 3 (1992),
p. 209-236

http://www.numdam.org/item?id=RO_1992__26_3_209_0

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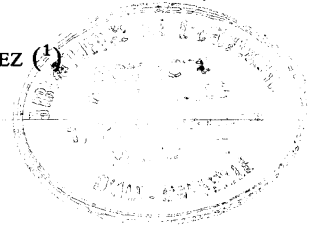
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NEW ALGORITHMS FOR MAXIMIZATION OF CONCAVE FUNCTIONS WITH BOX CONSTRAINTS (*)

by A. FRIEDLANDER ⁽¹⁾ and J. M. MARTINEZ ⁽¹⁾

Communicated by J. ABADIE



Abstract. — *This paper considers the problem of maximizing a differentiable concave function subject to bound constraints and a Lipschitz condition on the gradient, using active set strategies. A general model algorithm for this problem is proposed. The algorithm includes a procedure for deciding when to leave a face of the polytope without having reached a stationary point relative to that face, guaranteeing that return to that face excludes a neighborhood of fixed size of the current point. Mild conditions are required to abandon a face, which may possibly never be visited again, and we show that any face may be revisited at most a finite number of times. We show a bound for this quantity. We prove global convergence for this algorithm and we also show that it identifies the correct optimal face in a finite number of iterations, even without any nondegeneracy condition, when we use the "chopped gradient" introduced in [10], as the direction on which we leave any face. We combine the active set strategy proposed with a gradient projection method following the approach of Moré-Toraldo ([23, 24]), in order to accelerate the identification of the correct optimal face.*

Keywords : Optimization; box constraints.

Résumé. — *Nouveaux algorithmes pour la maximisation de fonctions concaves à variables bornées. Ce travail considère le problème de maximiser une fonction concave différentiable soumise à des restrictions de bornes sur les variables et dont le gradient satisfait aux conditions de Lipschitz, en utilisant une stratégie de restrictions actives. Un modèle d'algorithme général y est proposé pour le problème. L'algorithme contient un procédé permettant de décider, avant d'atteindre un point stationnaire d'une face, quand cette face du polytope doit être abandonnée, de façon à exclure un voisinage de grandeur fixe autour du point en question. Des conditions faibles sont nécessaires pour abandonner une face qui, probablement, ne sera jamais revisitée. Nous montrons : (i) qu'une face quelconque peut être revisitée un nombre fini des fois et, (ii) la valeur limite pour ce nombre. Dans ce travail la convergence globale de l'algorithme est démontrée. On montre aussi qu'il identifie correctement la face optimale en un nombre fini d'itérations, même sans aucune condition de non-dégénérescence, si la direction du « chopped » gradient est utilisée quand on abandonne la face [10]. Finalement, nous combinons la stratégie de restrictions actives avec la méthode de la projection du gradient, suivant l'approche de Moré-Toraldo ([23], [24]), de façon à accélérer l'identification correcte de la face optimale.*

Mots clés : Optimisation; restriction de bornes; projection du gradient.

(*) Received February 1990.

Work supported by F.A.P.E.S.P. (Grant 90-3724-6), F.I.N.E.P., CNPq and F.A.E.P.-U.N.I.C.A.M.P..

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1. INTRODUCTION

Many practical problems require the minimization of a convex C^1 -function with bound constrained variables:

$$(1.1) \quad \begin{cases} \text{Minimize } c(x) \\ \text{s. t. } l \leq x \leq u \end{cases}$$

where $c: \mathbb{R}^n \rightarrow \mathbb{R}$ is convex and has continuous first derivatives in the domain under consideration. For technical reasons, we will consider, instead of (1.1), the equivalent problem of maximizing a concave C^1 -function:

$$(1.2) \quad \begin{cases} \text{Maximize } f(x) \\ \text{s. t. } l \leq x \leq u \end{cases}$$

where $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is differentiable in the same sense as the function c of (1.1).

A very important particular case of (1.1) is the case where c is a convex quadratic. Applications of this case arise in finite difference discretization of free boundary problems [5, 27], numerical simulation of friction problems in rigid body mechanics [20], Image Reconstruction from projections [18], implementation of robust SQP-type methods for Nonlinear Programming [26], etc.

Many successful algorithms for solving (1.2) are based on active set strategies (*see* [2, 11, 12, 16, 27, 28]). Briefly speaking, an active set method proceeds generating iterates on a face of the polytope until either a maximum of the objective function on that face or a point on the boundary of the face is reached. In the second case, the algorithm continues working in a face of lower dimension, and only in the first case the iterates are allowed to abandon the current face and go on working in a face of higher dimension. Since function values are strictly increasing, finite convergence is obtained (*see* [27, 28]). However, these finite convergence results are based on the fact that a finite algorithm is available for finding a stationary point on a given face, when such a point exists. No algorithm with that property exists for general concave functions, and, even in the quadratic case, the use of conjugate gradient algorithms imposes utilization of convergence criteria for inner iterations different from the very exigent stationary point condition. O'Leary [27] suggests using empirically determined tolerance parameters ϵ_k in order to declare convergence of the inner iteration, but she does not give a theoretical justification for this device.

In a recent paper [10], Friedlander and Martínez introduced an active set algorithm for maximization of a concave function subject to bound constraints with the following characteristics: the criterion for leaving a face going to a higher dimension one does not assume that the current point is stationary relative to that face, but the next point is guaranteed to have a higher function value than the greatest function value on the old face. They proved that, after a finite number of iterations, all iterates lie on a face such that its closure contains an optimizer of the problem. Moreover, inside each face, any globally convergent algorithm for unconstrained problems may be used, so that the ultimate rate of convergence is the one of the unconstrained algorithm chosen.

This paper contains two essential improvements of the algorithm presented in [10]. First, instead of the criterion used in [10] for leaving a face, we require a milder condition which guarantees that no iteration after the current one belongs to a neighborhood of fixed size of the current iteration. Therefore, we are able to give a bound for the number of times each face is abandoned.

The second improvement is that, following the ideas of Moré and Toraldo [23, 24], we consider the polygonal path defined by the projection on the polytope of the half-line generated by the “escape direction”. Therefore, the active set may change dramatically from one iteration to the next one (see [6, 23, 24]), a fact that represents a positive advantage for large-scale problems. Moreover, a good “polygonal search” may guarantee that each face is visited (and abandoned) a small number of times.

We consider two possible “escape directions”. The first is the “chopped gradient” direction also considered in [10]. Using it we are able to prove a global convergence theorem and we also prove (without nondegeneracy conditions) that an optimal face is identified in a finite number of steps. The second “escape direction” is the classical projected gradient (see [1, 4, 15, 19, 22]). In this case we prove the same results as in the case of the “chopped gradient” but we need a nondegeneracy assumption. A third (minor) improvement of the algorithms presented in this paper over the one introduced in [10] is that here we use a more general model algorithm for searches inside each face. This model algorithm allows curvilinear or dogleg strategies (see [7]).

Notation

We use the following notation:

$\|\cdot\|$ is the 2-norm on $\mathbb{R}^n$.

$\langle \cdot, \cdot \rangle$ is the ordinary scalar product, $\langle x, y \rangle = x^T y$.

$(v)_i$ indicates the i -th component of a vector $v \in \mathbb{R}^n$.

$\#I$ is the number of elements of the set I .

2. THE NEW ALGORITHMS

General Hypotheses

We consider the problem of maximizing a continuously differentiable concave function with bound constrained variables:

$$(2.1) \quad \begin{cases} \text{Maximize } f(x) \\ \text{s. t. } x \in \Omega, \end{cases}$$

where $\Omega = \{x \in \mathbb{R}^n \mid l \leq x \leq u, l < u\}$.

Let us assume that g , the gradient of f , satisfies a Lipschitz condition in Ω :

$$(2.2) \quad \|g(x) - g(y)\| \leq L \|x - y\|, \quad \forall x, y \in \Omega$$

(2.2) implies that, for all $x, z \in \Omega$,

$$(2.3) \quad f(z) - f(x) - \langle g(x), (z - x) \rangle \geq -\frac{L}{2} \|z - x\|^2$$

(see [7]).

Let us define an open face of Ω as a set $F_I \subset \Omega$ such that

(2.4) I is a (possibly empty) subset of $\{1, 2, \dots, 2n\}$ such that i and $n+i$ cannot belong to I simultaneously, $i = 1, \dots, n$.

$$(2.5) \quad F_I = \{x \in \Omega \mid x_i = l_i \text{ if } i \in I, x_i = u_i \text{ if } n+i \in I, \\ l_i < x_i < u_i, \text{ otherwise}\}.$$

Therefore, the set Ω is divided into 3^n disjoint faces. Let us call $\bar{F}_I$, the closure of each open face, $[F_I]$ the smallest linear manifold which contains F_I , $\mathcal{S}(F_I)$ the parallel subspace to $[F_I]$ and $\dim F_I$ the dimension of $\mathcal{S}(F_I)$. Clearly, $\dim F_I = n - \#I$.

For each $x \in \Omega$ let us define $g_p(x)$ a real n -vector such that

$$(2.6) \quad \begin{aligned} (g_p(x))_i &= 0 && \text{if } x_i = l_i \text{ and } \frac{\partial f}{\partial x_i}(x) < 0 \\ & && \text{or } x_i = u_i \text{ and } \frac{\partial f}{\partial x_i}(x) > 0 \\ &= \frac{\partial f}{\partial x_i}(x), && \text{otherwise} \end{aligned}$$

Therefore, a necessary and sufficient condition for x being a global optimizer of our problem (see [13]) is:

$$(2.7) \quad g_p(x) = 0.$$

For each $x \in \bar{F}_I$ let us define $g_I(x)$ as

$$(2.8) \quad \begin{aligned} (g_I(x))_i &= 0 && \text{if } i \in I \text{ or } n+i \in I \\ &= \frac{\partial f}{\partial x_i}(x), && \text{otherwise} \end{aligned}$$

Therefore, $g_I(x)$ is the orthogonal projection of $g(x)$ on $\mathcal{S}(F_I)$. We also define, for $x \in \bar{F}_I$,

$$(2.9) \quad \begin{aligned} (g_I^c(x))_i &= 0 && \text{if } i \notin I \text{ and } n+i \notin I \\ &= 0 && \text{if } i \in I \text{ and } \frac{\partial f}{\partial x_i}(x) < 0 \\ & && \text{or } n+i \in I \text{ and } \frac{\partial f}{\partial x_i}(x) > 0 \\ &= \frac{\partial f}{\partial x_i}(x) && \text{otherwise.} \end{aligned}$$

The vector g_I^c plays a major role in the main results of this paper. We shall name it the "chopped gradient" associated with F_I . Clearly, for all $x \in \bar{F}_I$ we have

$$g_p(x) = g_I(x) + g_I^c(x)$$

LEMMA 2.1: Assume that $\bar{x} \in \bar{F}_I$ is such that

$$(2.10) \quad f(\bar{x}) \geq f(x) \text{ for all } x \in \bar{F}_I.$$

Then the two following statements are equivalent:

$$(2.11) \quad f(\bar{x}) \geq f(x) \quad \text{for all } x \in \Omega.$$

$$(2.12) \quad g_I^c(\bar{x}) = 0.$$

Proof: Let us assume (2.11). If $i \in I$, then $\bar{x}_i = l_i$, and so, by (2.6) and (2.7) $(\partial f / \partial x_i)(\bar{x}) \leq 0$. Analogously, if $n + i \in I$, then $\bar{x}_i = u_i$ and $(\partial f / \partial x_i)(\bar{x}) \geq 0$. Therefore, by (2.9), $g_I^c(\bar{x}) = 0$.

Now, assume (2.12). We want to prove that $g_p(\bar{x}) = 0$. For each $i = 1, \dots, n$, let us consider the following three possibilities:

$$(2.13) \quad \bar{x}_i = l_i,$$

$$(2.14) \quad \bar{x}_i = u_i,$$

$$(2.15) \quad l_i < \bar{x}_i < u_i.$$

Let us consider first (2.13). We have two alternatives:

$$(2.16) \quad i \in I,$$

$$(2.17) \quad i \notin I.$$

If (2.16) holds, we have, since $(g_I^c(\bar{x}))_i = 0$, and using (2.9), that $(\partial f / \partial x_i)(\bar{x}) \leq 0$. Therefore, by (2.6), $(g_p(\bar{x}))_i = 0$.

If $i \notin I$, then $x_i > l_i$ for all $x \in F_I$. But, by (2.10), $f(\bar{x}) \geq f(x)$ for all $x \in F_I$, therefore $(\partial f / \partial x_i)(\bar{x}) \leq 0$. So, $(g_p(\bar{x}))_i = 0$. The same argument leads to $(g_p(\bar{x}))_i = 0$, when $\bar{x}_i = u_i$.

Now, if (2.15) holds, we have, by (2.10), that $(\partial f / \partial x_i)(\bar{x}) = 0$. Thus, the desired result is proved. $\square$

In Lemma 2.1 we proved that a stationary point $\bar{x}$ for $\bar{F}_I$, either is a global optimizer in Ω , or has a nonnull $g_I^c(\bar{x})$. Thus, $g_I^c(\bar{x})$ should be a useful direction for escaping from a nonoptimal face.

We consider the mapping $P: \mathbb{R}^n \rightarrow \Omega$ such that:

$$\begin{aligned} (P(x))_i &= x_i & \text{if } l_i \leq x_i \leq u_i \\ &u_i & \text{if } x_i > u_i \\ &l_i & \text{if } x_i < l_i \end{aligned}$$

P is the projection of $\mathbb{R}^n$ onto Ω . Now, we are able to define the following algorithms:

ALGORITHM 2.1: Define

$$\gamma_I = \min \{u_i - l_i, i \in I \text{ or } n + i \in I\}$$

and

$$D_I = \text{diameter of } F_I$$

Let $M, \sigma, \theta, \alpha$ be given constants such that M is a positive integer, $0 < \sigma < 2/L$, $\theta, \alpha \in (0, 1)$. If $x^k \in F_I$ is the k -th approximation to a maximizer of f in Ω , and $g_p(x^k) \neq 0$, the steps for obtaining x^{k+1} are the following:

Step 1 (Test the location of the maximizer of a minorizing parabola and then test if the internal gradient is small enough).

Define $D = D_I/M$.

If

$$\|g_I^c(x^k)\| > L\gamma_I \quad \text{and} \quad \|g_I(x^k)\| < L\gamma_I^2/(2D)$$

or

$$\|g_I^c(x^k)\| \leq L\gamma_I \quad \text{and} \quad \|g_I(x^k)\| < \|g_I^c(x^k)\|^2/(2DL)$$

go to Step 2. Else, go to Step 3.

Step 2 (Find a feasible point outside $\bar{F}_I$ with a sufficient large function value). Compute $\lambda > 0$ such that

$$f(P(x^k + \lambda g_I^c(x^k))) > f(x^k) + \|g_I(x^k)\| D.$$

Set

$$x^{k+1} = P(x^k + \lambda g_I^c(x^k)). \quad \text{Stop.}$$

Step 3 (Test if the current point is near the boundary of F_I).

If $x^k + \sigma g_I(x^k) \notin F_I$, go to Step 6.

Step 4 (Determine an ascent direction for optimizing inside $\bar{F}_I$).

(i) Choose a direction $d_k \in \mathcal{S}(F_I)$ satisfying

$$(2.19) \quad \|d_k\| \geq \sigma \|g_I(x^k)\|$$

$$(2.20) \quad \langle d_k, g_I(x^k) \rangle \geq \theta \|d_k\| \|g_I(x^k)\|$$

[Observe that such a direction exists, for instance $\sigma g_I(x^k)$ satisfies (2.19), (2.20)]

(ii) If $x^k + d_k \in \Omega$, go to Step 5.

(iii) Compute

$$(2.21) \quad \bar{\lambda} = \max \{ \lambda \geq 0 \mid x^k + \lambda d_k \in \Omega \}.$$

(iv) Replace d_k by $\bar{\lambda} d_k$. If d_k satisfies (2.19), go to Step 5. Else set $d_k = g_I(x^k)$

(v) Compute $\bar{\lambda}$ by (2.21) replace d_k by $\bar{\lambda} d_k$.

Step 5 (Find a point inside $\bar{F}_I$ with a sufficient large function value)

(i) Let $s = d_k$

(ii) If

$$(2.22) \quad f(x^k + s) \geq f(x^k) + \alpha \langle g_I(x^k), s \rangle \quad \text{go to (iv)}$$

(iii) Choose $\bar{s} \in \mathcal{S}(F_I)$ such that

$$(2.23) \quad \langle \bar{s}, g_I(x^k) \rangle \geq \theta \|\bar{s}\| \|g_I(x^k)\|$$

and

$$(2.24) \quad 0.1 \|s\| \leq \|\bar{s}\| \leq 0.9 \|s\|$$

Let $s = \bar{s}$ and go to (ii).

(iv) Set $d_k = s$ and $x^{k+1} = x^k + d_k$. Stop.

Step 6 (Take a point on the boundary of F_I with a strictly larger function value).

Let $\bar{\lambda} = \max \{ \lambda \geq 0 \mid x^k + \lambda g_I(x^k) \in \Omega \}$ and set $x^{k+1} = x^k + \bar{\lambda} g_I(x^k)$. Stop.

The next algorithm is a variant of Algorithm 2.1 that uses $g_p(x^k)$ instead of $g_I^c(x^k)$ to escape from a nonoptimal face.

ALGORITHM 2.2: Let γ_I , D_I , M , σ , θ , α be as in Algorithm 2.1. Given $x^k \in F_I$ such that $g_p(x^k) \neq 0$, the steps for obtaining x^{k+1} are the following:

Step 0 (Test feasibility for steplength γ_I).

If $g_I^c(x_k) \neq 0$ and $x^k + \gamma_I g_p(x^k) / \|g_p(x^k)\| \in \Omega$, go to Step 1. Else go to Step 3.

Step 1

The same as in Algorithm 2.1 replacing $g_I^c(x^k)$ by $g_p(x^k)$

Step 2

Step 3 }
 Step 4 } The same as in Algorithm 2.1.
 Step 5 }
 Step 6 }

Remark: In Section 3, we prove that these algorithms are well defined. We also prove a convergence theorem for each algorithm and guarantee that the optimal active constraints are identified in a finite number of iterations. No additional hypotheses are required for Algorithm 2.1. For Algorithm 2.2 we shall need a nondegeneracy condition.

Now, we intend to shed some light on the meaning of the steps that define Algorithms 2.1 and 2.2.

Let us start with Step 1 of Algorithm 2.1. Consider the parabola defined by

$$\varphi(\lambda) = f(x^k) + \lambda \|g_I^c(x^k)\|^2 - \lambda^2 \frac{L}{2} \|g_I^c(x^k)\|^2.$$

Due to (2.3), we have for $\lambda \geq 0$

$$f(x^k + \lambda g_I^c(x^k)) \geq \varphi(\lambda)$$

The unconstrained maximizer of $\varphi(\lambda)$ is $\lambda = 1/L$, therefore in Step 1, we are testing first if $1/L < \gamma_I / \|g_I^c(x^k)\|$. We prove in Section 3, that in this case we guarantee that $x^k + (1/L) g_I^c(x^k)$ is feasible. If $1/L \geq \gamma_I / \|g_I^c(x^k)\|$, we take $\lambda = \gamma_I / \|g_I^c(x^k)\|$ in order to guarantee the feasibility of $x^k + \lambda g_I^c(x^k)$. Clearly, we have that

$$(2.25) \quad \varphi\left(\frac{1}{L}\right) = f(x^k) + \frac{1}{2L} \|g_I^c(x^k)\|^2$$

and

$$(2.26) \quad \varphi\left(\frac{\gamma_I}{\|g_I^c(x^k)\|}\right) = f(x^k) + \gamma_I \|g_I^c(x^k)\| - L \gamma_I^2 / 2.$$

We use (2.26) when $\|g_I^c(x^k)\| > L \gamma_1$. Then

$$(2.27) \quad \varphi\left(\frac{\gamma_I}{\|g_I^c(x^k)\|}\right) > f(x^k) + L \gamma_1^2 / 2$$

Thus, moving away from x^k in the direction of $g_I^c(x^k)$, we achieve improvements in the values of f of at least $(1/2L)\|g_I^c(x^k)\|^2$ or $L\gamma_I^2/2$ depending on the choice of λ . Now, if these values are greater than $\|g_I(x^k)\|D$, we may show (see Section 3, Lemma 3.3) that $f(x^k + \lambda g_I^c(x^k))$ is greater than $f(y)$, for every $y \in F_I$ such that $\|y - x^k\| \leq D$. So, if we satisfy any of the tests in Step 1, we go to Step 2. We will show in Section 3, that the required improvement ($\|g_I(x^k)\|D$) is possible. If $x^k + \sigma g_I(x^k) \notin F_I$ (see Step 3), we conclude that x^k is very near to the boundary of F_I , and thus, it is cheaper to take the next iterate in the boundary (Step 6) than to continue searching in F_I . We also show in Section 3, that this choice of x^{k+1} produces an improvement in the objective function value.

Finally, if the tests in Step 1 are not satisfied and x^k is not "near" to the boundary, we conclude that $\|g_I(x^k)\|$ is still large and therefore it is convenient to continue inside F_I . Thus, Steps 4 and 5 are executed. These steps consist in a quite general unconstrained optimization algorithm. We show in Section 3 that this algorithm "converges", so a sufficiently small value of $\|g_I(x^k)\|$ is always obtained, and consequently the face F_I is abandoned, unless it is an optimal face.

Algorithm 2.2 uses $g_p(x)$ instead of $g_I^c(x)$ and performs an additional Step 0. In this step, we test if $x^k + \gamma_I g_p(x^k)/\|g_p(x^k)\|$ is feasible. (This test is not necessary when using $g_I^c(x)$). In Section 3 we prove that under a nondegeneracy condition, we guarantee the feasibility of $x^k + \gamma_I (g_p(x^k)/\|g_p(x^k)\|)$, for a sufficiently large value of k , when working in a non optimal face. Once feasibility is obtained, all our assertions above remain valid if we replace $g_I^c(x^k)$ by $g_p(x^k)$.

3. CONVERGENCE RESULTS

In this section we prove the following theorems:

THEOREM 3.1: *Algorithms 2.1 and 2.2 are well-defined.*

THEOREM 3.2: *Any sequence $\{x^k\}$ generated by Algorithm 2.1 either stops at an iterate which is a global optimizer of (2.1), or, if infinite, satisfies*

(3.1) *There exists $I \subset \{1, \dots, 2n\}$, $k_0 \geq 0$, such that $x^k \in F_I$ for all $k \geq k_0$ and $\bar{F}_I$ contains a global optimizer of (2.1).*

(3.2) *Every limit point of $\{x^k\}$ is a global optimizer of (2.1).*

If $x \in \bar{F}_I$ is such that $g_I(x) = 0$, we shall call it a stationary point relative to F_I .

Assume that $x \in F_I$ is a stationary point relative to F_I . We say that x is non degenerate if $(\partial f / \partial x_i)(x) \neq 0$ whenever $x_i \in \{l_i, u_i\}$. Otherwise, we say that x is a degenerate stationary point.

For proving convergence of Algorithm 2.2 we will assume that the problem has no degenerate stationary points. Clearly, this assumption may be stated as follows:

Nondegeneracy Condition

For all $x \in \Omega$, if $x \in \bar{F}_I$ is a stationary point relative to F_I , then $x \in F_I$.

Assuming the nondegeneracy condition, we are able to prove the following global convergence theorem for algorithm 2.2:

THEOREM 3.3: Assume that problem (2.1) is such that for all $F_I \subset \Omega$, $F_I \neq \emptyset$, there are no degenerate stationary points relative to F_I . Then, any sequence $\{x^k\}$ generated by Algorithm 2.2, either stops at an iterate which is a global optimizer, or, if infinite, satisfies (3.1) and (3.2).

The proofs of Theorems 3.1, 3.2 and 3.3 are obtained as a consequence of the following lemmas:

LEMMA 3.1: Let $\gamma_I = \min \{u_i - l_i, i \in I \text{ or } n+i \in I\}$ and $x \in \bar{F}_I$ such that $g_I^c(x) \neq 0$. Define

$$(3.3) \quad \omega_I^c(x) = g_I^c(x) / \|g_I^c(x)\|.$$

Then

$$(3.4) \quad x + \gamma \omega_I^c(x) \in \Omega - \bar{F}_I \quad \text{for all } \gamma \in [0, \gamma_I].$$

Proof: It is sufficient to prove that

$$(3.5) \quad l_i \leq x_i + \gamma \omega_I^c(x) \leq u_i$$

for all $i \in \{1, \dots, n\}$, $\gamma \in [0, \gamma_I]$.

If $i \notin I$ and $n+i \notin I$, (3.5) is true since $(\omega_I^c(x))_i = 0$ by definition (2.9).

If $i \in I$, we have since $x \in \bar{F}_I$, that $x_i = l_i$. Therefore, by (2.9), either $(\omega_I^c(x))_i = 0$, or $(\omega_I^c(x))_i > 0$. In any case, by (3.3),

$$(3.6) \quad 0 \leq (\omega_I^c(x))_i \leq 1$$

Therefore,

$$l_i \leq l_i + \gamma (\omega_I^c(x))_i \leq l_i + \gamma_I \leq l_i + (u_i - l_i) \leq u_i.$$

If $(\omega_I^c(x))_i > 0$, then $l_i < l_i + \gamma(\omega_I^c(x))_i$ and so $x + \gamma\omega_I^c(x) \notin \bar{F}_I$.

A similar argument is used if $n+i \in I$, therefore $x + \gamma\omega_I^c(x) \in \Omega$. But, since $g_I^c(x) \neq 0$, some component of $\omega_I^c(x)$ is nonnull. So, $x + \gamma\omega_I^c(x) \notin \bar{F}_I$. This completes the proof. $\square$

LEMMA 3.2: Let $\bar{x} \in F_I$ be such that

$$(3.7) \quad g_I(\bar{x}) = 0$$

$$(3.8) \quad g_I^c(\bar{x}) \neq 0.$$

Define

$$(3.9) \quad \omega^p(x) = g_p(x) / \|g_p(x)\|.$$

Then, there exists $V(\bar{x})$, a neighborhood of $\bar{x}$ relative to F_I , such that

$$x + \gamma\omega^p(x) \in \Omega - \bar{F}_I \quad \text{for all } x \in V(\bar{x}) \text{ and } \gamma \in [0, \gamma_I].$$

Proof: Let

$$(3.10) \quad J = \{i \in \{1, 2, \dots, n\} \mid i \notin I \quad \text{and} \quad n+i \notin I\}$$

and

$$(3.11) \quad \delta_i(\bar{x}) = \min \{u_i - \bar{x}_i, \bar{x}_i - l_i\}.$$

Define

$$(3.12) \quad \varepsilon_J(\bar{x}) = \min \{\delta_i(\bar{x}), i \in J\}.$$

Clearly, since $\bar{x} \in F_I$, we have that $\varepsilon_J(\bar{x}) > 0$.

Now, $g_I(x)$ and $g_p(x)$ are continuous when restricted to F_I , therefore, by (3.7) and (3.8), there exists a neighborhood $V(\bar{x}) \subset F_I$ such that for all $x \in V(\bar{x})$

$$(3.13) \quad \|x - \bar{x}\| < \varepsilon_J(\bar{x})/2$$

and for all $i = 1, 2, \dots, n$

$$(3.14) \quad \gamma_I \left| \frac{(g_I(x))_i}{\|g_p(x)\|} \right| < \frac{\varepsilon_J(\bar{x})}{2}.$$

Now, we are able to show that if $x \in V(\bar{x})$

$$l_i \leq x_i + \gamma(\omega^p(x))_i \leq u_i$$

for all $i \in \{1, 2, \dots, n\}$, $\gamma \in [0, \gamma_I]$.

If $i \in J$, by the definitions (2.6), (2.8), (2.9),

$$x_i + \gamma (\omega^p(x))_i - l_i = x_i - l_i + \gamma (g_I(x))_i / \|g_p(x)\|.$$

From (3.12), (3.13) and (3.14) we obtain

$$x_i + \gamma (\omega^p(x))_i - l_i > 0 \quad \text{for } \gamma \in [0, \gamma_I].$$

The same argument leads to

$$u_i - (x_i + \gamma (\omega^p(x))_i) > 0 \quad \text{for } \gamma \in [0, \gamma_I].$$

Now, take $i \in I$. In this case

$$x_i + \gamma (\omega^p(x))_i = x_i + \gamma (g_I^c(x))_i / \|g_p(x)\|.$$

Therefore, we have that

$$\left| \frac{(g_I^c(x))_i}{\|g_p(x)\|} \right| < 1$$

So, the same arguments used in Lemma 3.1 lead to the desired result. $\square$

Remarks: $P(x + \lambda \omega_I^c(x))$ and $P(x + \lambda \omega^p(x))$ are linear functions of λ , on any interval on which the active set of $P(x + \lambda \omega_I^c(x))$ or $P(x + \lambda \omega^p(x))$, respectively, is unchanged. Both Lemma 3.1 and Lemma 3.2 state conditions under which the first interval includes $[0, \gamma_I]$.

We show later that we may obtain sufficient increase of the objective function in the direction $\omega_I^c(x)$ or $\omega^p(x)$ for a value of $\lambda \in [0, \gamma_I]$. The assumption that $\bar{x} \in F_I$ in Lemma 3.2 is restrictive. If $\bar{x} \in \bar{F}_I - F_I$ the thesis of Lemma 3.2 may not be true. Take, for example

$$f(x_1, x_2) = -\frac{1}{2}x_1^2 - \frac{1}{20}x_2^2$$

and $\Omega = \{x \in \mathbb{R}^2 \mid 0 \leq x_i \leq 10\}$. Then,

$$\nabla f(x) = \begin{pmatrix} -x_1 \\ -x_2/10 \end{pmatrix}$$

Consider the point $\bar{x} = \begin{pmatrix} 0 \\ 10 \end{pmatrix}$, and let

$$F_I = \{x \in \Omega \mid x_2 = 10\}, \quad \text{so } I = \{4\}, \quad \gamma_I = 10.$$

Then

$$\nabla f(\bar{x}) = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \quad g_I(\bar{x}) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad g_I^c(\bar{x}) = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

Now, consider points $x = \begin{pmatrix} x_1 \\ 10 \end{pmatrix}$ with $x_1 \rightarrow 0$. Obviously, there is no neighborhood of $\bar{x}$ in F_I such that for every x in that neighborhood, $x + \gamma\omega^p(x)$ is feasible for all $\gamma \in [0, \gamma_I]$. Note that $\begin{pmatrix} 0 \\ 10 \end{pmatrix}$ is a degenerate stationary point relative to $F_{\{1,4\}}$. This observation suggests that if we wish to consider problems with possibly degenerate stationary points in faces F_I , the direction given by $g_I^c(x)$ should be used.

LEMMA 3.3: Let $0 < D \leq D_I$, $0 < \lambda \leq \gamma_I$ and $x \in \bar{F}_I$ such that $g_I^c(x) \neq 0$. Then for all $y \in F_I$ such that $\|x - y\| \leq D$,

$$(3.15) \quad f(x + \lambda\omega_I^c(x)) - f(y) \geq \lambda \|g_I^c(x)\| - \left(\frac{L}{2}\right)\lambda^2 - \|g_I(x)\|D.$$

If $x + \lambda\omega^p(x) \in \Omega$, then assertion (3.15) is also true if we replace $\omega_I^c(x)$ by $\omega^p(x)$.

Proof: The concavity of f implies that for all $y \in F_I$ such that $\|x - y\| \leq D$

$$(3.16) \quad f(y) \leq f(x) + \langle g_I(x), y - x \rangle$$

and using the Cauchy-Schwarz inequality,

$$(3.17) \quad f(y) \leq f(x) + \|g_I(x)\|D.$$

Now, by (2.3), we have:

$$(3.19) \quad f(x + \lambda\omega_I^c(x)) - f(x) - \langle g(x), \lambda\omega_I^c(x) \rangle \geq -\frac{L}{2}\lambda^2,$$

and by the definition of $\omega_I^c(x)$,

$$(3.20) \quad f(x + \lambda \omega_I^c(x)) - f(x) - \lambda \|g_I^c(x)\| \geq -\frac{L}{2} \lambda^2$$

or

$$(3.21) \quad f(x + \lambda \omega_I^c(x)) - f(x) \geq \lambda \|g_I^c(x)\| - \frac{L}{2} \lambda^2$$

Subtracting (3.17) from (3.21) we obtain (3.15).

If we assume that $x + \lambda \omega^p(x) \in \Omega$, the proof of inequality (3.15) with $\omega^p(x)$ instead of $\omega_I^c(x)$ is exactly the same. $\square$

LEMMA 3.4: *If x^{k+1} is defined at Step 6 of Algorithms 2.1 or 2.2, then*

$$(3.22) \quad x^{k+1} \in F_J, \quad \text{where} \quad \dim(F_J) < \dim(F_I),$$

$$(3.23) \quad f(x^{k+1}) > f(x^k)$$

Proof: By the definition of $g_I(x)$ and $\bar{\lambda}$ at Step 6, x^{k+1} belongs to the boundary of F_I , therefore, (3.22) is true.

Let us prove (3.23). Since $x^k + \sigma g_I(x^k) \notin F_I$, we have $g_I(x^k) \neq 0$, and $0 < \bar{\lambda} \leq \sigma$.

Now, by (2.3), we have:

$$(3.24) \quad f(x^k + \bar{\lambda} g_I(x^k)) - f(x^k) - \bar{\lambda} \langle g(x^k), g_I(x^k) \rangle \geq -\left(\frac{L}{2}\right) \bar{\lambda}^2 \|g_I(x^k)\|^2$$

But

$$\langle g(x^k), g_I(x^k) \rangle = \langle g_I(x^k), g_I(x^k) \rangle = \|g_I(x^k)\|^2.$$

Hence, by (3.24)

$$f(x^k + \bar{\lambda} g_I(x^k)) - f(x^k) - \bar{\lambda} \|g_I(x^k)\|^2 \geq -\left(\frac{L}{2}\right) \bar{\lambda}^2 \|g_I(x^k)\|^2.$$

Therefore,

$$(3.25) \quad f(x^k + \bar{\lambda} g_I(x^k)) \geq f(x^k) + \left(\bar{\lambda} - \left(\frac{L}{2}\right) \bar{\lambda}^2\right) \|g_I(x^k)\|^2$$

But $\bar{\lambda} - (L/2) \bar{\lambda}^2 > 0$ for all $\bar{\lambda} \in (0, 2/L)$, and $0 < \bar{\lambda} \leq \sigma < 2/L$.

Thus by (3.25),

$$f(x^{k+1}) = f(x^k + \bar{\lambda} g_I(x^k)) > f(x^k)$$

and the desired result is proved. $\square$

Proof of Theorem 3.1: Let us consider first Algorithm 2.1. If $x^k \in F_I$ is not a solution of (2.1), x^{k+1} is defined either at Step 2, 5 or 6.

If x^{k+1} is defined at Step 2 we have that either

$$(3.26) \quad \frac{\|g_I^c(x^k)\|}{L} > \gamma_I \quad \text{and} \quad \frac{L\gamma_I^2}{(2D)} > \|g_I(x^k)\|$$

or

$$(3.27) \quad \|g_I^c(x^k)\| \leq \gamma_I L \quad \text{and} \quad \frac{\|g_I^c(x^k)\|^2}{(2DL)} > \|g_I(x^k)\|$$

By Lemma 3.1 we have that $x^k + \gamma_I \omega_I^c(x^k) \in \Omega - \bar{F}_I$. Then if (3.26) holds,

$$P(x^k + \gamma_I \omega_I^c(x^k)) = x^k + \gamma_I \omega_I^c(x^k),$$

and by (3.21) in Lemma 3.3 and (3.26),

$$\begin{aligned} f(P(x^k + \gamma_I \omega_I^c(x^k))) &\geq f(x^k) + \gamma_I \|g_I^c(x^k)\| - \frac{L}{2} \gamma_I^2 \\ &\geq f(x^k) + L \gamma_I^2 - \frac{L}{2} \gamma_I^2 = f(x^k) + \frac{L}{2} \gamma_I^2 \\ &\geq f(x^k) + \|g_I(x^k)\| D. \end{aligned}$$

If (3.27) holds, let us define $\lambda = \|g_I^c(x^k)\|/L$. By (3.21) and (3.27) we have:

$$P(x^k + \lambda \omega_I^c(x^k)) = x^k + \lambda \omega_I^c(x^k)$$

and

$$\begin{aligned} f(P(x^k + \lambda \omega_I^c(x^k))) &\geq f(x^k) + \|g_I^c(x^k)\|^2/L - \|g_I^c(x^k)\|^2/(2L) \\ &= f(x^k) + \|g_I^c(x^k)\|^2/(2L) \\ &> f(x^k) + \|g_I(x^k)\| D. \end{aligned}$$

Thus, we showed, that for $\lambda = \gamma_I$ or $\lambda = \|g_I^c(x^k)\|/L$ we may obtain the desired increase in the objective function.

If x^{k+1} is defined at Step 5, we are maximizing in F_I , and thus we require a sufficient increase condition of the Armijo's rule type using an ascent direction d_k . This condition is obviously satisfied if λ is small enough (see [7, 13]).

If x^{k+1} is defined at Step 6, by Lemma 3.4, it belongs to the boundary of F_I , and

$$f(x^{k+1}) > f(x^k).$$

The same results hold for Algorithm 2.2, replacing $\omega_I^c(x^k)$ by $\omega^p(x^k)$. $\square$

Remark: We do not need nondegeneracy conditions to guarantee that Algorithm 2.2 is well-defined. In fact, by Step 0 of this algorithm, the tests (3.26)-(3.27) (with g^p instead of g_I^c) for leaving a face are performed only if the segment $[x^k, x^k + \gamma_I \omega^p(x^k)]$ is contained in Ω . It is possible, when degeneracy is present, that this never happens, as in the counter-example which follows Lemma 3.2, and this will affect the convergence properties of the algorithm, but not its well-definition.

LEMMA 3.5: Assume that $x^k \in F_I$, and that $x^{k+j} \in F_I$ is computed for all $j \geq 1$ at Step 5 of algorithms 2.1 or 2.2. Then there exists a limit point $\bar{x}$ of the sequence $\{x^{k+j}\}_{j \geq 1}$, such that $\bar{x} \in \bar{F}_I$ and $g_I(\bar{x}) = 0$.

Proof: The sequence $\{x^{k+j}\}_{j \geq 1}$ is contained in $\bar{F}_I$, which is a compact subset of $\mathbb{R}^n$, so there exists a limit point $\bar{x} \in \bar{F}_I$.

If $g_I(x^{k+j}) = 0$ for some j , then by Lemma 3.2 we would have feasibility for stepsize γ_I in Algorithm 2.2, and consequently in both algorithms we would compute x^{k+j+1} at Step 2. Thus, our assumption implies that $g_I(x^{k+j}) \neq 0$ for all $j \geq 1$.

Now, we want to prove that $g_I(\bar{x}) = 0$. Let $\{x^{k+j_l}\}_{l \geq 1}$ be a subsequence of $\{x^{k+j}\}_{j \geq 1}$ such that

$$(3.28) \quad \lim_{l \rightarrow \infty} x^{k+j_l} = \bar{x}$$

By (2.22),

$$(3.29) \quad f(x^{k+j_l+1}) \geq f(x^{k+j_l}) + \alpha \langle g_I(x^{k+j_l}), d_{k+j_l} \rangle$$

and by (2.23), we have:

$$(3.30) \quad f(x^{k+j_l+1}) \geq f(x^{k+j_l}) + \alpha \theta \|g_I(x^{k+j_l})\| \|d_{k+j_l}\|$$

As $j_2 \geq j_1 + 1$, we have that

$$(3.31) \quad f(x^{k+j_2}) \geq f(x^{k+j_1}) + \alpha\theta \|g_I(x^{k+j_1})\| \|d_{k+j_1}\|$$

Repeating the same arguments, we get, in general, for $l > 1$:

$$(3.32) \quad f(x^{k+j_l}) \geq f(x^{k+j_1}) + \alpha\theta \sum_{s=1}^{l-1} \|g_I(x^{k+j_s})\| \|d_{k+j_s}\|$$

Now, by (2.19) in Step 4 and (2.22), (2.23), (2.24) in Step 5, we have the two following possibilities.

Case 1: $\|d_{k+j_l}\| \geq \sigma \|g_I(x^{k+j_l})\|$ for $t \in K_1$, K_1 an infinite subset of positive integers.

In this case we have

$$(3.33) \quad f(x^{k+j_t}) \geq f(x^{k+j_1}) + \alpha\theta\sigma \sum_{s=1}^{t-1} \|g_I(x^{k+j_s})\|^2.$$

(3.28) and the continuity of $f(x)$ imply that

$$(3.34) \quad f(\bar{x}) = \lim_{t \rightarrow \infty} f(x^{k+j_t}) \geq f(x^{k+j_1}) + \alpha\theta\sigma \sum_{s=1}^{\infty} \|g_I(x^{k+j_s})\|^2$$

then $\sum_{s=1}^{\infty} \|g_I(x^{k+j_s})\|^2$ converges and we have that

$$\lim_{s \rightarrow \infty} \|g_I(x^{k+j_s})\|^2 = 0.$$

By (3.28) and the continuity of $(\partial f / \partial x_i)(x)$ for all i we deduce that $g_I(\bar{x}) = 0$.

Case 2: $\|d_{k+j_l}\| < \sigma \|g_I(x^{k+j_l})\|$ for all $l \geq l_0$.

Now, we get for $l \geq l_0$ in inequation (3.32):

$$(3.35) \quad f(x^{k+j_l}) \geq f(x^{k+j_{l_0}}) + \frac{\alpha\theta}{\sigma} \sum_{s=l_0}^{l-1} \|d_{k+j_s}\|^2.$$

Taking limits with $l \rightarrow \infty$, we obtain

$$(3.36) \quad f(\bar{x}) \geq f(x^{k+j_{l_0}}) + \sum_{s=l_0}^{\infty} \|d_{k+j_s}\|^2.$$

So, $\sum_{s=l_0}^{\infty} \|d_{k+j_s}\|^2$ converges and

$$(3.37) \quad \lim_{s \rightarrow \infty} \|d_{k+j_s}\| = 0.$$

We also have in this case, by (2.22), (2.23) and (2.24) in Step 5, that there exists $s_{k+j_l} \in \mathcal{S}(F_I)$, such that

$$(3.38) \quad 0 < \|s_{k+j_l}\| \leq 10 \|d_{k+j_l}\| \quad \text{for } l \geq l_0,$$

$$(3.39) \quad \langle s_{k+j_l}, g_I(x^{k+j_l}) \rangle \geq \theta \|s_{k+j_l}\| \|g_I(x^{k+j_l})\|,$$

and

$$(3.40) \quad f(x^{k+j_l} + s_{k+j_l}) < f(x^{k+j_l}) + \alpha \langle g_I(x^{k+j_l}), s_{k+j_l} \rangle$$

(3.37) and (3.38) imply that

$$(3.41) \quad \lim_{l \rightarrow \infty} \|s_{k+j_l}\| = 0.$$

The sequence $\{s_{k+j_l}/\|s_{k+j_l}\|\}$ is contained in the unit sphere, so it must have a limit point. So, there exists an infinite subset $K_2 \subset \{l \geq l_0\}$ such that

$$(3.42) \quad \lim_{l \in K_2} \frac{s_{k+j_l}}{\|s_{k+j_l}\|} = v \quad \text{with } \|v\| = 1.$$

Now, by, (3.40), for $l \in K_2$,

$$\frac{f(x^{k+j_l} + s_{k+j_l}) - f(x^{k+j_l})}{\|s_{k+j_l}\|} < \frac{\alpha \langle g_I(x^{k+j_l}), s_{k+j_l} \rangle}{\|s_{k+j_l}\|}$$

and by the Mean Value Theorem,

$$\frac{\langle g_I(x^{k+j_l} + \xi_k s_{k+j_l}), s_{k+j_l} \rangle}{\|s_{k+j_l}\|} < \frac{\alpha \langle g_I(x^{k+j_l}), s_{k+j_l} \rangle}{\|s_{k+j_l}\|}$$

with $\xi_k \in [0, 1]$.

Now, making $l \rightarrow \infty$, with $l \in K_2$ we obtain, by (3.41) and (3.42), that

$$(3.43) \quad \langle g_I(\bar{x}), v \rangle \leq \alpha \langle g_I(\bar{x}), v \rangle.$$

But $\langle g_I(\bar{x}), v \rangle \geq 0$ by (3.39) and $\alpha \in (0, 1)$ by definition. So (3.43) is possible only if

$$\langle g_I(\bar{x}), v \rangle = 0.$$

But as $\|v\| = 1$, we necessarily have $g_I(\bar{x}) = 0$. Thus, the proof is complete. $\square$

LEMMA 3.6: Assume that $\bar{F}_I$ does not contain a global optimizer of problem (2.1) and that $x^k \in F_I$. Then:

- (i) After a finite number of steps j of Algorithm 2.1, $x^{k+j} \notin F_I$.
- (ii) If we assume that every stationary point relative to F_I is nondegenerate then assertion (i) is also true for Algorithm 2.2.

Proof: If (i) is not true, then $x^{k+j} \in F_I$ is computed at Step 5 for all $j \geq 1$. By Lemma 3.5, we know that the sequence $\{x^{k+j}\}_{j \geq 1}$ has a limit point $\bar{x} \in \bar{F}_I$ such that $g_I(\bar{x}) = 0$. Our assumption on $\bar{F}_I$ implies that $g_I^c(\bar{x}) \neq 0$ and $g_p(x) \neq 0$. By the definition of $g_I^c(x)$ and the continuity of the gradient of f in Ω , we deduce that there exist $\varepsilon, \delta > 0$ such that for all $x \in F_I$ with $\|x - \bar{x}\| < \delta$, we have $\|g_I^c(x)\| > \varepsilon$ and $\|g_p(x)\| > \varepsilon$. Then, for sufficiently large j , we shall meet points x^{k+j} satisfying the conditions required in Step 1. So, x^{k+j+1} will be computed at Step 2 for these points. This is a contradiction, so part (i) of our lemma is proved.

Let us prove part (ii). If we assume that (i) is false, we have, as before, a limit point $\bar{x} \in \bar{F}_I$, of $\{x^{k+j}\}_{j \geq 1} \subset F_I$, such that $g_I(\bar{x}) = 0$ and $g_I^c(\bar{x}) \neq 0$. Now, by the Nondegeneracy Condition, we know that $\bar{x} \in F_I$, and by Lemma 3.2, there exists $V(\bar{x})$ a neighborhood of $\bar{x}$, $V(\bar{x}) \subset F_I$ such that $x + \gamma_I \omega_p(x) \in \Omega - \bar{F}_I$ for all $x \in V(\bar{x})$. So, for sufficiently large j , feasibility will be obtained at Step 0 of Algorithm 2.2, and from then on, we shall always go to Step 1. Now, the same arguments used to prove (i) for Algorithm 2.1 are valid for Algorithm 2.2. This completes the proof. $\square$

So far, we proved that the following assertion is true for Algorithm (2.1):

Algorithm (2.1) stops after a finite numbers of iterations k , finding a global solution of (2.1), or it generates an infinite sequence which satisfies the following properties:

$$(3.44) \quad f(x^{k+1}) > f(x^k) \quad \text{for all } k = 0, 1, 2, \dots$$

$$(3.45) \quad \text{Given } x^k \in F_I, \text{ one and only one of three following possibilities holds:}$$

$$(3.45a) \quad x^{k+1} \in F_I.$$

$$(3.45b) \quad x^{k+1} \in F_J \quad \text{where } \dim(F_J) < \dim(F_I).$$

(3.45 c) $x^{k+1} \notin \bar{F}_I$ and $f(x^{k+1}) > f(x)$ for all $x \in F_I$ such that $\|x - x^k\| \leq D$

(3.46) If $x^k \in F_I$ and $\bar{F}_I$ does not contain a global optimizer of (2.1), then there exists $l > k$ such that $x^l \notin F_I$.

(3.44) and (3.45) are also true for Algorithm 2.2. If we assume the Nongeneracy Condition, then by Lemma 3.6, (3.46) is also true for Algorithm 2.2. Let us prove now that (3.44), (3.45), (3.46) are sufficient conditions to prove that an Algorithm identifies in a finite numbers of steps a face F_I such that a solution of problem (2.1) is in $\bar{F}_I$.

LEMMA 3.8: Assume that a sequence $\{x^k, k \in \mathbb{N}\}$ satisfies (3.44)-(3.46). Then, there exists a positive integer l_0 such that for all $k > l_0$, either (3.45 a) or (3.45 b) holds.

Proof: Suppose, on the contrary, that there exists an infinite set of indexes K such that for $l \in K$, x^{l+1} verifies (3.45 c).

We may find an infinite subset $K_1 \subset K$, such that $x^j \in F_J$ for all j in K_1 and some fixed set J . (The number of faces F_I is finite). Then we have, by (3.45 c) that for $j \in K_1$, $x^{j+1} \notin F_J$ and $f(x^{j+1}) > f(x)$ for all $x \in F_J$ such that $\|x - x^j\| \leq D$.

Let $j, m \in K_1$ such that $m > j$. Then, by (3.44) and (3.45 c), we have

$$(3.47) \quad f(x^m) \geq f(x^{j+1})$$

and

$$(3.48) \quad f(x^{j+1}) > f(x) \quad \text{for all } x \in F_J \text{ such that } \|x - x^j\| \leq D$$

(3.47) and (3.48) imply that $\|x^m - x^j\| > D$.

So, the sequence $\{x^j\}$ with $j \in K_1$, is an infinite subset of the compact set $\bar{F}_J$, such that the distance between two arbitrary elements is greater than a fixed value $D > 0$. This is impossible, so there exists l_0 with the desired property. $\square$

LEMMA 3.9: Let us assume again (3.44)-(3.46). If $\bar{F}_I$ does not contain a global optimizer of (2.1) then there exists $k_I > 0$ such that $x^k \notin F_I$ for all $k \geq k_I$.

Proof: Let l_0 be as in Lemma 3.8. We have two possibilities:

$$(3.49) \quad x^k \notin F_I \quad \text{for all } k \geq l_0.$$

$$(3.50) \quad \text{There exists } k > l_0 \text{ such that } x^k \in F_I.$$

Suppose that (3.50) holds.

By (3.46), we may take j as the first index such that $j > k$ and $x^j \notin F_I$.

By (3.50) $j-1 > l_0$ and by Lemma 3.8 we have that

$$x^j \in F_J \quad \text{where} \quad \dim(F_J) < \dim(F_I)$$

and that for $m > j$ either $x^m \in F_J$ or $x^m \in F_{J_m}$ where $\dim(F_{J_m}) < \dim F_J$. Then, the desired result is obtained taking $k_I = \max\{l_0, j\}$. $\square$

LEMMA 3.10: *Under the same assumptions of Lemmas 3.8 and 3.9, there exists $m_0 > 0$, such that if $k \geq m_0$, $x^k \in \bigcup F_I$ such that $\bar{F}_I$ contains a global optimizer of (2.1).*

Proof: Take $m_0 = \max\{k_I\}$, k_I as in Lemma 3.9. $\square$

Proof of Theorem 3.2: Suppose that the sequence is infinite. By Lemma 3.8 and Lemma 3.10, if $k_1 = \max\{l_0, m_0\}$ we have that for all $k \geq k_1$

$$x^k \in \bigcup F_I \text{ such that } \bar{F}_I \text{ contains a global optimizer of (2.1).}$$

Let $x^{k_1} \in F_{k_1}$.

If $x^k \in F_{k_1}$ for all $k \geq k_1$, take $k_0 = k_1$ and we are done.

If $x^{k_2} \notin F_{k_1}$ for some index $k_2 > k_1$, by Lemma 3.8, we have that

$$x^{k_2} \in F_{k_2} \quad \text{where} \quad \dim(F_{k_2}) < \dim(F_{k_1}).$$

Continuing this reasoning, as the number of different faces F_I is finite, and the sequence infinite, we must stop with k_i such $x^k \in F_{k_i}$ for all $k \geq k_i > \dots > k_2 > k_1$ and $\dim F_{k_i} \geq 1$.

So (3.1) is true with $k_0 = k_i$ and $F_I = F_{k_i}$.

By Lemma 3.5, we have that $g_I(\bar{x}) = 0$ for any limit point of $\{x^k\}$. Now, our function is concave and $\bar{F}_I$ contains a global optimizer. Then $g_I(\bar{x}) = 0$ and so, $\bar{x}$ is a global optimiser of (2.1).

So, the desired result is proved. $\square$

Proof of Theorem 3.3: If we assume that Nondegeneracy Condition, by Lemma 3.6, Algorithm 2.2 has the properties (3.44), (3.45) and (3.46). Thus, the proof of this theorem is the same as the proof of Theorem 3.2. $\square$

Remarks: (i) We proved in Lemma 3.6 that if $x^k \in F_I$ such that there is no global optimizer in $\bar{F}_I$, there exists $j_0 \geq 1$ such that $x^{k+j_0} \notin F_I$. That is, after a finite number of steps of the algorithms, we leave F_I . If j_0 is such that $x^{k+j_0-1} \in F_I$, we guarantee that the intersection of a ball centered in x^{k+j_0-1} with radius $D/2$ and F_I is never revisited. Let us call $\eta = \dim F_I = n - \#F_I$. The union of all the balls with center in F_I and radius $D/2$ is contained in

the set

$$\mathcal{F} = \left\{ x \in \mathbb{R}^n \mid x_i = l_i \text{ if } i \in I, x_i = u_i \text{ if } n+i \in I, \right. \\ \left. l_i - \frac{D}{2} < x_i < u_i + \frac{D}{2} \text{ otherwise} \right\}.$$

The η -dimensional volume of $\mathcal{F}$ is

$$\text{Vol}(\mathcal{F}) = \prod_{\substack{i \in I \\ n+i \notin I}} (u_i - l_i + D)$$

But the η -dimensional volume of each ball of radius $D/2$ restricted to F_I is greater than $(D/2)^\eta \eta^{-\eta/2}$. Therefore, the number of iterates $x^k \in F_I$ such that $x^{k+1} \notin \bar{F}_I$, is less than or equal to

$$\begin{aligned} \text{MAX} &= \prod_{\substack{i \notin I \\ n+i \notin I}} (u_i - l_i + D) / [(D/2)^\eta \eta^{-\eta/2}] \\ &\leq [\max_{\substack{i \notin I \\ n+i \notin I}} (u_i - l_i + D)]^\eta / [(D/2)^\eta \eta^{-\eta/2}] \\ &= \left[\frac{2(D_I + D) \eta^{1/2}}{D} \right]^\eta = [2(M+1) \eta^{1/2}]^\eta. \end{aligned}$$

Of course, it is expected than in practical computations the number of these type of steps will be much less than the bound above. However, the possibility of obtaining such a bound, independent of f , l and u is interesting from the theoretical point of view.

(ii) We showed that with the direction $g_I^c(x^k)$, there is no need of the nondegeneracy hypothesis in order to obtain our convergence results. Moreover, if we use $g_I^c(x^k)$ when we try to leave face F_I , the free variables remain unchanged and that the stepsize γ_I is always feasible. Thus, to compute the new point it is sufficient to consider the changes of components with indices i such that $i \in I$ or $n+i \in I$. In other words, the number of "break points" of the polygonal path is $\sim \#I$ when we use g_I^c and grows to $\sim n$ when g_p is used. Consequently, Algorithm 2.1 is in practice much simpler than Algorithm 2.2, which uses direction $g_p(x^k)$.

(iii) Lemma 3.3 guarantees the existence of a value of λ , such that sufficient increase is obtained in Step 2. In practice, of course, we shall not necessarily use this theoretically guaranteed value. An adequate line search

strategy should provide us with a value of λ satisfying the sufficient increase condition. The theoretical value gives us a better point on the first piece of the linear piecewise path defined by $P(x^k + \lambda g_I^c(x^k))$. This comes from relaxing some constraints without adding any new constraint. We expect that with other values of λ , we should be able also to add constraints, improving the performance of the algorithm.

4. NUMERICAL EXPERIENCE

The numerical performance of Algorithms 2.1 and 2.2 is highly dependent on the choice of d_k at Step 4. Our main interest is the resolution of large scale problems, so we used the Fletcher-Reeves conjugate gradient formula (see [8], p. 65) in our computer implementation. We use $\sigma \leq 10^{-4}$, $\theta = 10^{-6}$ in the safeguarding inequalities (2.19) and (2.20). If any of these inequalities is not satisfied by the Fletcher-Reeves direction, we replace d_k by $g_I(x^k)$.

With the above choice of d_k , the storage requirements of the algorithms 2.1 and 2.2 are very low. So, we were able to solve many large scale optimization problems within a very modest computer environment (IBM PC-XT type microcomputer with 640 Kb of RAM).

The optimum value of M depends on the characteristics of the problem. In general, we obtained the best results with $M \approx 100$, but in many cases the choice $M=1$ was more efficient. Remember that when $M=1$, the current face is abandoned only when returning to it is impossible. On the other hand setting $M \geq 100$ produces a mild condition for leaving the face.

Our practical experience with Algorithms 2.1 and 2.2 comes from four types of problems.

1. *Problems of optimal operation policy of hydro-thermal energy generation* (See [9, 21])

This type of problems gives rise to large-scale highly structured nonlinear programs with bounds and linear constraints. For running our methods it is necessary to transform these problems into box constrained problems via penalization of the equality constraints. Augmented Lagrangean techniques can also be used. Several techniques were used for solving these problems, that take advantage of the sparsity pattern of the technology matrix. In particular, we used the package MINOS of Stanford University (See [25]) and other active set methods of reduced gradient type, like the ones introduced by Friedlander *et al.* [9] and Gomes and Martínez [16]. As expected, when the

number of variables is not very large, so that the storage of the PC computer is sufficient to run the algorithms of [25, 9, 16], these algorithms are more efficient than the ones introduced in this paper due to the difficulties that are inherent to penalization. However, when the number of variables is very large, penalization is the only possible approach and algorithms like the ones described here become the only viable techniques. In [21] it is described an algorithm that can be considered an ancestor of the ones studied in this paper, where it can be observed that this approach can be extremely efficient for practical very large dynamic control problems.

2. Randomly generated linearly constrained large-scale problems with staircase structure

In [16] a set of large scale randomly generated nonlinear programming problems with linear constraints is described, where the technology matrix has staircase structure. The algorithms introduced in this paper can be used for solving these problems by means of penalization or augmented Lagrangean techniques, as so happens to be with the dynamic control problems mentioned above.

For this set of problems, the conclusions are the same as for the first set. In fact, MINOS is the most efficient technique for small to medium scale problems, and the algorithm of Gomes and Martínez is more efficient from medium to large scale problems. However, both MINOS and the Gomes-Martínez method are impracticable for very large problems where only penalization together with box constrained techniques can be used.

3. Physical problems

Many variational problems originated in the modellization of physical phenomena give rise to large-scale box constrained optimization problems (See [14]). We ran several variations of Algorithms 2.1 and 2.2 for solving the problem of finding the equilibrium position of an elastic membrane which passes through a curve Γ (Obstacle Problem [6, 24]). In these problems the best performance for Algorithms 2.1 and 2.2 was obtained using a large value of M ($M \approx 10,000$) and the algorithm 2.2 behaved slightly better than the algorithm 2.1 in terms of execution time. In general, our results are slightly better than those reported by Dembo and Tulowitzki [6], and comparable to the ones of Moré and Toraldo [24]. We are preparing a computer-oriented report where a detailed description of these experiments will be given.

4. *Box constrained problems with a random quadratic as objective function*

This set of problems is described in [23]. They are very useful for testing the effect of dual degeneracy in the performance of the algorithms. As expected, we observed that the performance of Algorithms 2.2 deteriorates in relation to Algorithm 2.1 in the presence of degeneracy. As in the previous case, the detailed results of these experiments will be showed in a forthcoming computer-oriented paper.

5. FINAL REMARKS

In the last few months we have been elaborating a production code based on a combination of Algorithms 2.1 and 2.2. Many colleagues and students tested preliminary versions of this code for solving Mathematical Programming and Physical problems. Up to the present, the code based on the techniques introduced in this paper has proved to be extremely robust. Our implementation is oriented towards the resolution of large-scale problems, so the speed in the resolution in small to medium problems was sacrificed in order to obtain reliable results for large problems.

However, the theoretical-based criterion for leaving the face described in this paper can be used in combination with other unconstrained techniques that are more suitable for problems of moderate size (Newton or Variable Metric). Many library subroutines for box constrained problems of moderate size have a built-in heuristic criterion for leaving the face. Any of these routines can be modified in order to incorporate our theoretically justified procedure, thus providing stronger justifications for convergence and, probably, better computational results at least in the presence of degeneration.

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