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RESEARCH ON AN AUGMENTED LAGRANGIAN PENALTY FUNCTION ALGORITHM FOR NONLINEAR PROGRAMMING

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Principal Investigator: Dr. Les Frair

Department of IEOR

VPI & SU

ABSTRACT

This research represents an extensive study of the Augmented Lagrangian (ALAG) Penalty Function Algorithm for optimizing nonlinear mathematical models. The mathematical models of interest are deterministic in nature and finite dimensional optimization is assumed. A detailed review of penalty function techniques in general and the ALAG technique in particular is presented. Numerical experiments are conducted utilizing a number of nonlinear optimization problems to identify an efficient ALAG Penalty Function Technique for computer implementation.

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I. INTRODUCTION

The current advanced stage of development of the theoretical framework of unconstrained optimization has served as a powerful force for unification of the subject which, until some years ago, consisted of a collection of disjointed algorithms. The evolution of these algorithms depended strongly on practical computation of solution to specific problems. The interplay of theory and algorithms has made it possible to transfer theoretical progress into improved algorithms.

Powell (P5) has reviewed comprehensively modern algorithms and the effect of theoretical work on the design of practical algorithms for unconstrained optimization. Murray (M11) has presented the mainstream of developments in numerical methods for unconstrained optimization. Much of the current research has been focused on understanding, comparing, improving and extending the available numerical methods instead of devising totally new algorithmic concepts. These refinements and modifications are not expected to significantly improve the efficiency of existing algorithms (G2).

At present a robust collection of potent and sophisticated general purpose algorithms for unconstrained optimization is available as high-quality software (G2). These algorithms have been tested and proven to be efficient and reliable for solving a variety of typical test problems and practical problems. Successful development of such algorithms for unconstrained optimization has been the springboard for the more recent success in the design of algorithms for constrained problems.

Availability of efficient numerical methods for solving unconstrained optimization problems has motivated the design of algorithms that convert a constrained problem to a sequence of unconstrained problems which have the property that successive solutions of the unconstrained problems converge to the solution of the constrained problem. This transformation approach has been systematically employed in the development of numerical algorithms for constrained optimization for more than a decade. In recent years a substantial body of theory has been established for these transformation techniques and many computational algorithms have been proposed (B4), (F1), (L3).

To review briefly the transformation technique, consider the following inequality constrained nonlinear programming problem. Let $f(\underset{\sim}{X})$ and $c_i\ (\underset{\sim}{X})$ $i = 1,2,....,m$ be real valued functions of class $C^{(2)}$ on a nonempty open set L in an n-dimensional Euclidean space E^n .

P1 : Minimize $f\ (\underset{\sim}{X})$ over all $\underset{\sim}{X} \varepsilon L$

Subject to $c_i\ (\underset{\sim}{X}) \geqq 0,\ i = 1,2,....,m$

where feasible region F is a nonempty compact set.

$$F = \{\underset{\sim}{X} : c_i\ (\underset{\sim}{X}) \geqq 0 \quad i = 1,2,....,m,\ \underset{\sim}{X} \varepsilon L,\ L \subseteq E^n\}$$

Methods for solving P1 via unconstrained minimization have been classified, described and analyzed in detail by Lootsma (L3). Parametric transformation methods solve P1 by reducing the computational process to a sequence of successive unconstrained minimizations of a compound function defined in terms of the objective function $f\ (\underset{\sim}{X})$, the constraint functions c_i $(\underset{\sim}{X})$ i = 1,2,....,m and one or more controlling parameters. By gradually removing the effect of the constraints in the compound function by controlled changes in the value of one or more parameters a sequence of unconstrained problems is generated. Successive solutions of these unconstrained problems converge to a solution of the original constrained problem. The advantage of this approach lies in the fact that the constraints need not be dealt with separately and that efficient numerical methods for computing unconstrained extrema can be applied.

During recent years the parametric transformation technique known as the Augmented Lagrangian (ALAG) Penalty Function Technique has gained recognition as one of the most effective type of methods for solving constrained minimization problems. In the opinion of many researchers in this field, the ALAG penalty function technique is the best method available for solving problems with nonlinear constraints in the absence of special structure (B4). The disadvantages of the method are negligible and the advantages are strong, especially the lack of numerical difficulties and the ease of using the unconstrained minimization routine. The method has global convergence at an ultimately superlinear rate, the computational effort per minimization falls off rapidly, initial starting point need not be feasible and the function is defined for all values of the parameters (F7).

The ALAG penalty function technique is a balance between the classical penalty function technique and the Lagrangian primal-dual method which are both parametric transformation techniques. The design of this method was motivated by efforts to overcome the numerical instability of the penalty function technique near the solution (P3), (H2) and attempts to eliminate the "duality gap" in nonconvex programming (R6). The classical penalty function technique and the Lagrangian primal-dual method are briefly reviewed and the development of the ALAG penalty function technique by the merger of the penalty idea with the primal-dual philosophy is traced in section 2. The ALAG penalty function technique is described, reviewed and discussed in section 3. The results of numerical investigations are presented in section 4. The symbols, mathematical terms and related concepts used in this work are defined briefly in appendix A. The method of solving a nonlinear problem using the ALAG penalty function technique is illustrated with numerical examples in appendix B.

II. REVIEW OF RELATED MINIMIZATION TECHNIQUES

2.1 Penalty Function Technique

The penalty methods have been extensively used in numerical optimization for more than a decade. The penalty function approach has been popular, as evidenced by applications to practical problems (D3), because it is conceptually simple and easy to implement. It permits a transparent program structure as it is fully based on unconstrained minimization. These methods are applicable to a broad class of problems, even those involving nonconvex constraints. The most attractive feature of these methods is the fact that they take advantage of the powerful unconstrained minimization methods that have been developed in recent years.

The penalty function technique is a sequential parametric transformation method. It is an iterative algorithm that requires the solution of an unconstrained optimization problem at each iteration. In these methods the objective function $f(\underset{\sim}{X})$ is minimized using an unconstrained minimization technique while maintaining implicit control over the constraint violations by penalizing the objective function at points which violate or tend to violate the constraints. The solution $\underset{\sim}{X}^*$ to the constrained minimization problem P1 is approached from outside the feasible region F and these methods are also referred to as exterior point methods. The penalty function technique has been popularized mainly through the work of Fiacco and McCormick (F1). Fiacco and McCormick (F1) developed the Sequential Unconstrained Minimization Techniques (SUMT) for nonlinear programming using penalty function and related concepts. A chronological survey of the development of the penalty methods and detailed discussion and analysis of penalty and related methods are presented in reference (F1).

The penalty function method for P1 consists of sequential minimizations of the form

$$\text{minimize } P(\underset{\sim}{X}, \sigma), \quad \underset{\sim}{X} \in L \subseteq E^n$$

$P(\underset{\sim}{X}, \sigma)$ is the penalty function with control parameter $\sigma > 0$. This function is designed to impose an increasing penalty on the objective function as constraint violation increases. The control parameter σ is used effectively to increase the magnitude of penalty.

The penalty function transformation may be represented as

$$P(\underset{\sim}{X}, \sigma) = f(\underset{\sim}{X}) + \sigma \sum_{i=1}^{m} \eta_i(c_i(\underset{\sim}{X})), \quad \sigma > 0 \text{ where} \qquad [1]$$

$\eta_i(t)$ is defined as the loss function with the following properties.

(i) $\eta_i(t)$ is continuous on $-\infty < t < \infty$

(ii) for inequality constraint $c_i(\underset{\sim}{X}) \geqq 0$

$\eta_i(t) \to \infty$ as $t \to -\infty$ and $\eta_i(t) = 0$ for $t \geqq 0$

(iii) for equality constraint $c_i(\underset{\sim}{X}) = 0$

$\eta_i(t) \geqq 0 \; \forall t$, $\eta_i(t) = 0$ for $t = 0$ and

$\eta_i(t) \to \infty$ as $t \to \pm\infty$

Usually the loss function, $\eta_i(t)$, is chosen such that when the objective function and the constraint functions are of class $C^{(2)}$, $P(\underset{\sim}{X}, \sigma)$ is twice differentiable. $P(\underset{\sim}{X}, \sigma)$ is defined on an open set $L \subseteq E^n$ and $P(\underset{\sim}{X}, \sigma) \to \infty$ as constraint violation increases.

Several different loss functions have been proposed for use in the penalty function algorithm and these are discussed by Fiacco and McCormick

(F1). The most commonly and widely used loss function is the quadratic loss function. For an inequality constraint $c_i(\underset{\sim}{X}) \geqq 0$, quadratic loss function is $\eta_i(c_i(\underset{\sim}{X})) = [\min\,(0,\ c_i(\underset{\sim}{X}))]^2$. For an equality constraint $c_i(\underset{\sim}{X}) = 0$, the quadratic loss function is $\eta_i(c_i(\underset{\sim}{X})) = (c_i(\underset{\sim}{X}))^2$.

An elaborate treatment of the penalty function algorithm can be found in (F1), (L5) and (Z1) for a general nonlinear problem. The basic algorithm may be represented as follows:

(i) Select an infinite sequence $\{\sigma^{(k)}\}$ which is monotonically increasing as $k \to \infty$. Find $\underset{\sim}{X}^{(0)} \notin F$, where F is the feasible region defined by the constraint functions. Set $k = 0$.

(ii) Set $k = k + 1$.

(iii) Minimize $P(\underset{\sim}{X},\ \sigma^{(k)})$ to find $\underset{\sim}{X}(\sigma^{(k)}) = \underset{\sim}{X}^{(k)}$ starting the minimization from $\underset{\sim}{X}^{(k-1)}$. Return to (ii) if convergence is not satisfied.

Convergence tests in step (iii) are usually based on the magnitude of quantities such as $(f(\underset{\sim}{X}^{(k)}) - f(\underset{\sim}{X}^{(k-1)}))$ and $\| \underset{\sim}{X}^{(k)} - \underset{\sim}{X}^{(k-1)} \|$ where $\| \underset{\sim}{X} \|$ is the Euclidean norm of the vector $\underset{\sim}{X}$. Other convergence criteria are discussed by Fiacco and McCormick (F1). It is assumed that the function $f(\underset{\sim}{X})$ is bounded below so that a solution $\underset{\sim}{X}^{(k)}$ to the unconstrained minimization in step (iii) exists for each $\sigma^{(k)}$. In step (i) the initial starting point $\underset{\sim}{X}^{(0)}$ is outside the feasible region F and the trajectory corresponding to the sequence $\{\underset{\sim}{X}^{(k)}\}$ generated by the algorithm lies outside F. Therefore penalty function methods are also known as exterior-point methods. Any limit point of the sequence $\{\underset{\sim}{X}^{(k)}\}$ generated by the penalty method is a solution $\underset{\sim}{X}^*$ to the constrained minimization problem P1 (H4), (L5), (Z1).

The penalty function technique might be regarded as a "primal" approach to implicitly account for the constraints, although its connections with duality are known (F1), (L5), (Z1). The approximation of the constrained problem by the unconstrained penalty problem becomes more and more exact as the control parameter $\sigma \to \infty$. However considerable computational difficulties are experienced with the traditional penalty function algorithm as $\sigma \to \infty$. These difficulties are delineated in detail in references (L3), (L5), (M5), (R11). The computational difficulties arise from $P(\underset{\sim}{X}, \sigma)$ forming an increasingly steep-sided valley as the control parameter is increased to allow the unconstrained solutions to approach the constrained solution to P1 from outside the active constraints. In particular, the Hessian matrix of the penalty function [1] becomes extremely ill-conditioned as σ increases. This leads to numerical instabilities during unconstrained minimizations of the penalty function and slow convergence of the algorithm.

Attempts to overcome these computational difficulties have resulted in several modifications (F1), (F2), (L3) to the penalty function technique. Hestenes (H2) and Powell (P3), at about the same time, independently proposed modifications that resulted in a new method related to the penalty function technique. In this new method penalty terms are added to the Lagrangian associated with the original constrained problem. Hestenes (H2) termed this the "Multiplier Method". It has become known as the Augmented Lagrangian Penalty Function Technique in subsequent discussions. This method alleviated some of the computational difficulties associated with the traditional penalty function technique (F8) and achieved better convergence properties than the method of penalty functions (H4). This method is reviewed briefly in Chapter 3.

2.2 Lagrangian Primal-Dual Method

The Lagrangian primal-dual method transforms a constrained convex programming problem into a sequence of unconstrained minimizations of the classical Lagrangian associated with the constrained minimization problem. The constrained problem P1 becomes a convex programming problem when the objective function $f(\underset{\sim}{X})$ is convex and the constraints $c_i(\underset{\sim}{X})$ $i = 1, 2, \ldots, m$ are concave. The concept of the primal-dual method was first implemented by Arrow, et al. (A1) in the differential gradient scheme for approaching the saddle-point of the Lagrangian $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ associated with a convex program. The Lagrangian associated with the convex problem P1 may be represented as

$$L(\underset{\sim}{X}, \underset{\sim}{\lambda}) = f(\underset{\sim}{X}) - \sum_{i=1}^{m} \lambda_i \, c_i(\underset{\sim}{X}), \quad \underset{\sim}{X} \in \mathcal{L} \subseteq E^n, \quad \underset{\sim}{\lambda} \in E_+^m \qquad [2]$$

where E_+^m is the nonnegative orthant of m-dimensional Euclidean space E^m and the vector $\underset{\sim}{\lambda} \in E_+^m$ is called a vector of multipliers.

Suppose that a point $\underset{\sim}{X}^*$ satisfies the constraints of the convex program P1 and the problem functions are of class $C^{(1)}$. If there exists a vector $\underset{\sim}{\lambda}^*$ such that

$$\underset{\sim}{\lambda}^* \geqq 0, \quad \lambda_i^* \, c_i(\underset{\sim}{X}^*) = 0 \;\forall\; i \text{ and } \underset{\sim}{\nabla} L(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*) = 0, \qquad [3]$$

then $\underset{\sim}{X}^*$ is a global solution to the convex program P1. The vector $\underset{\sim}{\lambda}^*$ is said to be the vector of Lagrange multipliers associated with $\underset{\sim}{X}^*$. If the gradients of the active constraints at $\underset{\sim}{X}^*$ are linearly independent, then $\underset{\sim}{X}^*$ is a regular point of the feasible region $\mathcal{F}$ and there exists a vector of Lagrange multipliers $\underset{\sim}{\lambda}^*$ satisfying [3]. The conditions in [3] are called the Kuhn-Tucker first-order necessary conditions for $\underset{\sim}{X}^*$ to be a solution to

P1 and for the convex program P1, these are also sufficient conditions for $\underset{\sim}{X}^*$ to be a global solution. For a nondifferentiable convex problem P1 let there exist an $\underset{\sim}{X}^* \varepsilon E^n$ and a $\underset{\sim}{\lambda}^* \varepsilon E_+^m$ such that the pair $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ is the saddle-point of the Lagrangian $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ associated with the convex program P1, i.e., $L(\underset{\sim}{X}^*, \underset{\sim}{\lambda}) \leqq L(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*) \leqq L(\underset{\sim}{X}, \underset{\sim}{\lambda}^*)$. Then $\underset{\sim}{X}^*$ is the global solution to the convex program P1 and $\underset{\sim}{\lambda}^*$ is the vector of Lagrange multipliers associated with $\underset{\sim}{X}^*$.

The differential gradient scheme of Arrow, et al. (A1) for a convex program may be viewed as a small-step primal-dual method where estimates of $\underset{\sim}{X}^*$ and $\underset{\sim}{\lambda}^*$ are modified at each iteration to exploit the saddle-point nature of $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ near $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$. This structure of the method is revealed by the system of difference equations formulated by Uzawa (A1) to represent the differential gradient method. Davis (D1) represents the iterations in this method as

$$\underset{\sim}{X}^{(k+1)} = \underset{\sim}{X}^{(k)} - \alpha_1 B_1^{-1} \underset{\sim}{\nabla} L(\underset{\sim}{X}^{(k)}, \underset{\sim}{\lambda}^{(k)})$$

$$\underset{\sim}{\lambda}^{(k+1)} = \min [0, \underset{\sim}{\lambda}^{(k)} - \alpha_2 B_2^{-1} \underset{\sim\sim}{\nabla\lambda} L(\underset{\sim}{X}^{(k)}, \underset{\sim}{\lambda}^{(k)}]$$

where α_1 and α_2 are scalars representing step-size, $\underset{\sim}{\nabla} L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ is the gradient of $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ with respect to $\underset{\sim}{X}$, $\underset{\sim\sim}{\nabla\lambda} L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ is the gradient of $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ with respect to $\underset{\sim}{\lambda}$ and B_1^{-1} and B_2^{-1} are positive definite matrices of order n and m respectively. The algorithm may be started at any $\underset{\sim}{X}^{(0)} \varepsilon F$ and $\underset{\sim}{\lambda}^{(0)} \varepsilon E_+^m$.

As the constrained problem in the above method is convex, the Lagrangian $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ is also convex with respect to $\underset{\sim}{X}$. The iterations on $\underset{\sim}{X}^{(k)}$, therefore, are descent iterations on $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ and update of multipliers

$\underset{\sim}{\lambda}^{(k)}$ may be viewed as ascent iterations on $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$. The $\underset{\sim}{\lambda}^{(k)}$ update may also be regarded as approximate solutions to the associated dual problem at $\underset{\sim}{X}^{(k)}$. The dual associated with P1 is

$$\text{D1:}\quad \text{Maximize } \mathcal{V}(\underset{\sim}{\lambda}) \text{ over all } \underset{\sim}{\lambda} \in E_{+}^{m}$$

$$\mathcal{V}(\underset{\sim}{\lambda}) = \underset{\underset{\sim}{X}}{\text{infimum}}\ L(\underset{\sim}{X}, \underset{\sim}{\lambda}),\ \underset{\sim}{X} \in \mathcal{L}\,.$$

The Lagrangian $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ is minimized over $\underset{\sim}{X} \in \mathcal{L}$ for a sequence of multiplier vectors $\underset{\sim}{\lambda}^{(k)}$ and the algorithm is a primal-dual method. Methods that are similar in concept to this algorithm are described by Powell (P4), Bertsekas (B4), and Lasden (L1).

The algorithms based on Lagrangian primal-dual method are not susceptible to numerical instabilities such as those discussed in connection with the penalty method. Primal-dual methods are based on the viewpoint that the Lagrange multipliers $\underset{\sim}{\lambda}^*$ are also fundamental unknowns associated with a constrained problem. This is due to the reason that Lagrange multipliers measure sensitivities and often have meaningful interpretations as prices associated with constraint resources (H4), (L5). Useful duality results for convex programs have been presented by Luenberger (L5) and Zangwill (Z1). Various formulations of the duality theory for nonlinear convex programs using the classical Lagrangian have been reworked and extended by Geoffrion (G1) so as to facilitate, more readily, computational and theoretical applications. Methods based on the classical Lagrangian for solving a constrained problem P1 have been reviewed by Lootsma (L3).

The Lagrangian primal-dual method is known to have serious disadvantages (R3), (R6). The most restrictive one is that the constrained problem must be convex in order for the dual problem to be well defined and $\underset{\sim}{\lambda}$ iterations to be meaningful. In general inf (P1) $\geqq$ sup (D1) and the equality holds good only for the convex problem P1. For nonconvex problems only the inequality holds in the above relationship and in such cases a duality gap is said to exist. For nonconvex problems Everett (E2) introduced a primal dual method called generalized Lagrange multiplier method. This and other associated methods are summarized by Lootsma (L3). Even though Everett (E2) suggested some methods of handling the duality gap, the method has been found to be useful only for certain nonlinear problems with special structure. The method is of importance in the decompoisition of large-scale problems with separable functions. In such cases minimization of the Lagrangian can be carried out efficiently due to the special structure of the constrained problem (E2), (L1), (L5).

For a convex program, if $\underset{\sim}{X}^*$ is the optimal solution to the constrained problem with corresponding Lagrange multiplier vector $\underset{\sim}{\lambda}^*$, then $\underset{\sim}{X}^*$ is the unconstrained minimizer of $L(\underset{\sim}{X}, \underset{\sim}{\lambda}^*)$. However, if $\underset{\sim}{X}^*$ is a local solution to a nonconvex program with corresponding Lagrange multiplier vector $\underset{\sim}{\lambda}^*$, then $\underset{\sim}{X}^*$ may not be the unconstrained local minimizer of $L(\underset{\sim}{X}, \underset{\sim}{\lambda}^*)$ and $L(\underset{\sim}{X}, \underset{\sim}{\lambda}^*)$ may even have negative second derivatives at $\underset{\sim}{X}^*$ in certain directions normal to the feasible manifold F (R3). Since curvature at a point is determined by the second partial derivatives, attempts were made to make the Lagrangian associated with nonconvex programs a convex function by adding quadratic penalty terms to it. This concept was first suggested by Arrow and Solow (A1) in connection with the solution of a nonconvex equality constrained problem using the differential gradient method. Arrow and Solow augmented the classical Lagrangian with quadratic penalty terms and this elegant idea made the new augmented Lagrangian locally convex. This idea was independently reconsidered in an entirely different algorithmic context for equality constrained problems by Hestenes (H2), Powell (P3) and Haarhoff and Buys (H1). The algorithms that resulted from these efforts belong to the Augmented Lagrangian Penalty Function Technique which is reviewed in Section 3.

III. AUGMENTED LAGRANGIAN PENALTY FUNCTION TECHNIQUE

3.1 Introduction

The ALAG penalty function technique may be reviewed from two entirely different points of view. The first view-point is that the methods that belong to this technique modify the Lagrangian associated with a nonconvex or a weakly convex constrained problem to have a local convexity property. This is because the characterization of solution to a constrained problem in terms of a saddle-point of the Lagrangian depends heavily on convexity properties of the underlying problem. The local saddle-point property is obtained by the presence of a convexifying parameter in the Lagrangian which makes the associated Hessian positive definite for large enough, but finite, values of the parameter. Following this idea of local convexification many different modifications of the classical Lagrangian have been proposed to close the duality gap in nonconvex programming (A1), (A2), (M2).

The second viewpoint is to consider the technique and the quadratic penalty function method within a common generalized penalty function framework. The approach here is to circumvent instabilities associated with the classical penalty function method by adding penalty terms to the Lagrangian function. The advantages of using a first-order penalty furnction have been listed by Lootsma (L3) and McCormick (M5). Therefore methods that augment the Lagrangian with quadratic penalty terms are considered in detail. The development of the ALAG penalty function technique is traced from the second viewpoint.

3.2 Review of the Technique for Equality Constrained Problem

3.2.1 Equality Constrained Problem

The equality constrained problem P2 may be represented as follows:

$$\text{P2:}\quad \text{Minimize } f(\underset{\sim}{X})$$

$$\text{Subject to}\quad c_i(\underset{\sim}{X}) = 0 \quad i = 1, 2, \ldots, m \quad m \leqq n$$

$f(\underset{\sim}{X})$ and $c_i(\underset{\sim}{X})$ $i = 1, 2, \ldots, m$ are real-valued functions of class $C^{(2)}$ defined on a nonempty open set $\mathcal{L} \subseteq \mathcal{E}^n$. The Lagrangian associated with P2 is

$$L(\underset{\sim}{X}, \underset{\sim}{\lambda}) = f(\underset{\sim}{X}) - \sum_{i=1}^{m} \lambda_i \, c_i(\underset{\sim}{X}), \ \underset{\sim}{\lambda} \in \mathcal{E}^m. \qquad [4]$$

The gradient and Hessian of this Lagrangian with respect to $\underset{\sim}{X}$ are $\nabla L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ and $\nabla^2 L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ respectively.

Let $\underset{\sim}{X}^*$ be an optimal solution to P2 and the problem functions $f(\underset{\sim}{X})$ and $c_i(\underset{\sim}{X})$, $i = 1, 2, \ldots, m$ be of class $\mathcal{C}^{(2)}$ in an open neighborhood of $\underset{\sim}{X}^*$. The following are assumed to hold good at $\underset{\sim}{X}^*$.

(i) The point $\underset{\sim}{X}^*$ is a regular point of the feasible set

$\mathcal{F} = \{\underset{\sim}{X}: \ c_i(\underset{\sim}{X}) = 0 \ \ i = 1, 2, \ldots, m, \ \underset{\sim}{X} \in \mathcal{L} \subseteq \mathcal{E}^n\}$

Let $N^* = N(\underset{\sim}{X}^*)$ be the nxm matrix $[\underset{\sim}{\nabla c}_1, \underset{\sim}{\nabla c}_2, \ldots, \underset{\sim}{\nabla c}_m]$.

The regularity of the feasible set at $\underset{\sim}{X}^*$ is satisfied when N^* is of full rank.

(ii) There exists an unique Lagrange multiplier vector $\underset{\sim}{\lambda}^*$ such that the following first-order necessary conditions for local optimality at $\underset{\sim}{X}^*$ are satisfied.

$$\underset{\sim}{\lambda}^* \in \mathcal{E}^m, \ c_i(\underset{\sim}{X}^*) = 0 \ \forall i \text{ and } \nabla L(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*) = 0. \qquad [5]$$

(iii) The second-order necessary conditions for local optimality at $\underset{\sim}{X}^*$ are that in addition to [5]

$$\underset{\sim}{Y}^T \nabla^2 L(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*) \underset{\sim}{Y} \geqq 0 \quad \forall \underset{\sim}{Y} \in \mathcal{Y} \subseteq E^n \qquad [6]$$

$$\dot{\mathcal{Y}} = \{\underset{\sim}{Y}: \quad \underset{\sim}{Y}^T \nabla \underset{\sim}{c}_i = 0 \quad \forall i\}$$

(iv) The second-order sufficient conditions for $\underset{\sim}{X}^*$ to be an isolated local minimum are that in addition to [5]

$$\underset{\sim}{Y}^T \nabla^2 L(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*) \underset{\sim}{Y} > 0 \quad \forall \text{ nonzero } \underset{\sim}{Y} \in \mathcal{Y} \qquad [7]$$

(v) Strict complementarity holds at $\underset{\sim}{X}^*$, i.e., $\lambda_i^* \neq 0 \quad \forall i$

3.2.2 Powell - Hestenes Augmented Penalty Function

Powell (P3) suggested the following penalty function to solve P2.

$$\phi(\underset{\sim}{X}, \underset{\sim}{\theta}, S) = f(\underset{\sim}{X}) + \frac{1}{2} \sum_{i=1}^{m} \sigma_i (c_i(\underset{\sim}{X}) - \theta_i)^2$$

$$= f(\underset{\sim}{X}) + \frac{1}{2} (\underset{\sim}{c}(\underset{\sim}{X}) - \underset{\sim}{\theta})^T S \, (\underset{\sim}{c}(\underset{\sim}{X}) - \underset{\sim}{\theta}) \qquad [8]$$

where $\underset{\sim}{\theta} \in E^m$, $\underset{\sim}{C}(\underset{\sim}{X})$ is a vector of constraint functions $c_i(\underset{\sim}{X})$ $i = 1, 2, \ldots, m$ and S is a diagonal matrix of order m with diagonal elements $\sigma_i > 0$. Let $\underset{\sim}{\sigma} \in E^m_{++}$ be a vector with σ_i as components. While the classical penalty function for P2 contains at most m control parameters, the above function depends on 2m parameters which are the components of $\underset{\sim}{\theta}$ and $\underset{\sim}{\sigma}$. The main difference between classical quadratic penalty function and [8] is the introduction of parameters $\underset{\sim}{\theta}$. In [8] quadratic penalty terms have been added to the Lagrangian associated with P2.

The augmented penalty function ϕ is used in the algorithm as follows.

Algorithm A1:

```
(i)   Select $\underset{\sim}{\theta}^{(1)} = 0$,  $k = 0$,  $S^{(1)} = I$ and $\underset{\sim}{X}^{(0)} \notin \mathcal{F}$.
(ii)  $k = k + 1$
(iii) Minimize $\phi(\underset{\sim}{X}, \underset{\sim}{\theta}^{(k)}, S^{(k)})$ to find
          $\underset{\sim}{X}^{(k)} = \underset{\sim}{X}(\underset{\sim}{\theta}^{(k)}, S^{(k)})$ starting the unconstrained
      minimization from $\underset{\sim}{X}^{(k-1)}$.
(iv)  If $\underset{\sim}{C}(\underset{\sim}{X}^{(k)})$ is converging sufficiently rapidly to zero then
          $\underset{\sim}{\theta}^{(k+1)} = \underset{\sim}{\theta}^{(k)} - \underset{\sim}{C}(\underset{\sim}{X}^{(k)})$
          $S^{(k+1)} = S^{(k)}$ and return to (ii)
      otherwise
          $\underset{\sim}{\theta}^{(k+1)} = (1/10)\ \underset{\sim}{\theta}^{(k)}$
          $S^{(k+1)} = 10\ S^{(k)}$ and return to (ii).
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In step (ii) ϕ is minimized with respect to $\underset{\sim}{X}$ without constraints for fixed values of $\underset{\sim}{\theta}^{(k)}$ and $S^{(k)}$ and this is the inner iteration of the algorithm. Step (iii) is the outer iteration in which $\underset{\sim}{\theta}^{(k)}$ and $S^{(k)}$ are changed to force constraint satisfaction and cause the sequence of solutions $\{\underset{\sim}{X}^{(k)}\}$ to converge to $\underset{\sim}{X}^*$ at a reasonably fast rate.

The scheme for adjusting $\underset{\sim}{\theta}$ parameters in the outer iteration is based on the observation that if $\underset{\sim}{X}^{(k)}$ is the minimizer of $\phi(\underset{\sim}{X}, \underset{\sim}{\theta}^{(k)}, S^{(k)})$ in the inner iteration, then $\underset{\sim}{X}^{(k)}$ is also a solution of the problem

$$\text{Minimize } f(\underset{\sim}{X}) \qquad \underset{\sim}{X} \in \mathcal{L} \subseteq \mathcal{E}^n$$

$$\text{Subject to } \underset{\sim}{C}(\underset{\sim}{X}) = \underset{\sim}{C}(\underset{\sim}{X}^{(k)})$$

In order to solve the equality constrained problem P2 it is sufficient to find $\underset{\sim}{\theta}^{(k)}$ and $S^{(k)}$ such that $\underset{\sim}{X}^{(k)} = \underset{\sim}{X}(\underset{\sim}{\theta}^{(k)}, S^{(k)})$ solves the system of nonlinear equations

$$\underset{\sim}{C}(\underset{\sim}{X}(\underset{\sim}{\theta}^{(k)}, S^{(k)})) = 0. \qquad [9]$$

The above system of equations is in terms of 2m parameters θ_i and σ_i $i = 1, 2, \ldots, m$. One vector of parameters $\theta^{(k)}$ or $\sigma^{(k)}$ may be fixed and [9] then is a system of m equations in m remaining parameters.

If $\underset{\sim}{\theta}^{(k)}$ is fixed, then [8] reduces to a basic penalty transformation. Specifically when $\underset{\sim}{\theta}$ parameters are set to zero, ϕ becomes the classical quadratic penalty function. In such a case convergence of the sequence $\{\underset{\sim}{X}^{(k)}\}$ to $\underset{\sim}{X}^*$ is ensured by letting $\sigma_i \to \infty$, $i = 1, 2, \ldots, m$. This leads to numerical instabilities and slow convergence. Therefore in Powell's method $S^{(k)}$ is held constant and $\underset{\sim}{\theta}^{(k)}$ is changed to force constraint satisfaction through iterative solution of [9]. Powell (P2) derived a simple correction for adjusting $\underset{\sim}{\theta}^{(k)}$ parameters when $S^{(k)}$ is fixed by applying generalized Newton iteration to solve [9]. This correction is represented as

$$\underset{\sim}{\theta}^{(k+1)} = \underset{\sim}{\theta}^{(k)} - \underset{\sim}{C}(\underset{\sim}{X}^{(k)}). \qquad [10]$$

By definition $\underset{\sim}{X}^{(k)}$ is the unconstrained minimizer of $\phi(\underset{\sim}{X}, \underset{\sim}{\theta}^{(k)}, S^{(k)})$. Therefore $\underset{\sim}{\nabla}\phi(\underset{\sim}{X}^{(k)}, \underset{\sim}{\theta}^{(k)}, S^{(k)}) = 0$, i.e.,

$$\underset{\sim}{\nabla} f(\underset{\sim}{X}^{(k)}) + \sum_{i=1}^{m} \sigma_i (C_i(\underset{\sim}{X}^{(k)}) - \theta_i^{(k)}) \, \underset{\sim}{\nabla} C_i(\underset{\sim}{X}^{(k)}) = 0. \qquad [11]$$

Continuity of $\underset{\sim}{C}(\underset{\sim}{X})$ in the neighborhood of the local minimizer $\underset{\sim}{X}^*$ of P2 implies that the matrix $N(\underset{\sim}{X}^{(k)})$ is of full rank for $\underset{\sim}{X}^{(k)}$ sufficiently close to $\underset{\sim}{X}^*$. When $\underset{\sim}{X}^{(k)}$ is in the neighborhood of $\underset{\sim}{X}^*$ and when $\underset{\sim}{X}^{(k)} \to \underset{\sim}{X}^*$ the estimates

$$\underset{\sim}{\lambda}^{(k)} = -S^{(k)} \, (\underset{\sim}{C}(\underset{\sim}{X}^{(k)}) - \underset{\sim}{\theta}^{(k)}) \qquad [12]$$

exist and have as limit points the unique values $\underset{\sim}{\lambda}^* = S^* \underset{\sim}{\theta}^*$, where $\underset{\sim}{\theta}^*$ and S^* are the parameters corresponding to $\underset{\sim}{X}^*$. Hence the final value of the product $S \underset{\sim}{\theta}$, in the limiting sense, is a constant and may considered to be independent of S when S is fixed and $\underset{\sim}{\theta}$ is adjusted to let $\underset{\sim}{\theta} \to \underset{\sim}{\theta}^*$. Due to this reason, when S is increased in step (iii) of algorithm A1 to improve the rate of convergence of the sequence $\{\max_i |c_i(\underset{\sim}{X}^{(k)})|\}$ to 0 and $\{\underset{\sim}{X}^{(k)}\}$ to $\underset{\sim}{X}^*$, $\underset{\sim}{\theta}$ is decreased to keep $S \underset{\sim}{\theta}$ a constant.

Convergence of the algorithm is measured using the sequence $\{\max_i |c_i(\underset{\sim}{X}^{(k)})|\}$. Under the assumptions in 3.2.1 and when the Hessian matrix of ϕ is positive definite at $\underset{\sim}{X}^*$, Powell (P2) proved that the rate of convergence is linear and the convergence ratio depends on $1/\sigma_i$ for $\sigma_i \geqq \sigma'$. The threshold value σ' is a large but finite positive real number. Therefore by choosing S to be large so that S is close to S', where $S' = \sigma' I$, the algorithm can be made to have linear convergence at any arbitrary rate. Superlinear convergence is achieved when $\sigma_i \to \infty$. In Powell's algorithm the rate of convergence is taken to be satisfactory when the maximum residual, $\max_i |c_i(\underset{\sim}{X}^{(k)})|$, of the system of equations [9] is reduced by a factor of four on each iteration. The reason for preferring the slower rate of convergence implied by the use of factor four is that faster convergence tends to make the inner iterations more difficult (P2). When the sequence $\{\max_i |c_i(\underset{\sim}{X}^{(k)})|\}$ either fails to converge or converges to zero at too slow a rate, S is increased by a factor of ten. The choice of factor ten to increase S is arbitrary. Numerical evidence indicates that the value of σ_i is seldom required to be greater than 10^2 to ensure rapid convergence (R11).

The Hessian matrix of ϕ depends on both $\underset{\sim}{\theta}$ and S. The change in this matrix is dominated by the increase in S (P2). This is another reason for using a factor of ten to increase S when the rate of convergence is slow and keeping S constant when rate of convergence is satisfactory. If S is chosen to be large in the initial iteration, instead of gradually increasing S, the Hessian of ϕ becomes ill-conditioned and the unconstrained minimization of ϕ in the inner iteration becomes very difficult to perform. Further for a large S, an arbitrary starting point $\underset{\sim}{X}^{(0)}$ and arbitrary values of $\underset{\sim}{\theta}$ parameters, the sequence $\{\underset{\sim}{X}^{(k)}\}$ may not converge to $\underset{\sim}{X}^*$. Therefore S is increased so as to force $\underset{\sim}{X}^{(k)}$ into a region in which sequence $\{\underset{\sim}{X}^{(k)}\}$ locally converges to $\underset{\sim}{X}^*$. Once this region is reached, S is kept constant and $\underset{\sim}{\theta}$ parameters are adjusted so as to let $\underset{\sim}{X}^{(k)} \rightarrow \underset{\sim}{X}^*$. Further the gradual increase of S is designed to make ϕ continuous and continuously differentiable with respect to $\underset{\sim}{X}$ for all values of the parameters. In Powell's algorithm the minimizations in the inner iteration are not beset by computational difficulties associated with the basic penalty function transformations. The minimizations are well scaled and progressively less computational effort is required as k increases and $\underset{\sim}{X}^{(k)} \rightarrow \underset{\sim}{X}^*$.

Hestenes (H2), independently of Powell and at about the same time, proposed a similar method for solving P2 and he called it the method of multipliers. The method is based on the observation that if $\underset{\sim}{X}^*$ is a nonsingular minimum of P2, there exists a multiplier vector $\underset{\sim}{\lambda}^*$ and a constant σ such that $\underset{\sim}{X}^*$ affords an unconstrained local minimum to the function

$$T(\underset{\sim}{X}, \underset{\sim}{\lambda}^*, S) = f(\underset{\sim}{X}) - \underset{\sim}{\lambda}^{*T} \underset{\sim}{C}(\underset{\sim}{X}) + 1/2 \, (\underset{\sim}{C}(\underset{\sim}{X}))^T S\underset{\sim}{C}(\underset{\sim}{X}) \qquad [13]$$

where S = σI. Conversely, if $\underset{\sim}{C}(\underset{\sim}{X}^*) = 0$ and $\underset{\sim}{X}^*$ affords a minimum to [13], then $\underset{\sim}{X}^*$ affords a minimum to P2. In the method of multipliers a large positive constant σ is suitably chosen and is held fast. The augmented penalty function considered is

$$T(\underset{\sim}{X}, \underset{\sim}{\lambda}, S) = f(\underset{\sim}{X}) - \underset{\sim}{\lambda}^T \underset{\sim}{C}(\underset{\sim}{X}) + 1/2 \; (\underset{\sim}{C}(\underset{\sim}{X}))^T \; S\underset{\sim}{C}(\underset{\sim}{X}) \qquad [14]$$

where $\underset{\sim}{\lambda} \varepsilon \mathcal{B}$ and $\mathcal{B}$ is an arbitrary compact subset of $\mathcal{E}^m$. The function in [14] is sequentially minimized for successive estimates $\underset{\sim}{\lambda}$ of the unique Lagrange multiplier vector $\underset{\sim}{\lambda}^*$ at $\underset{\sim}{X}^*$.

The unconstrained minimization of $T(\underset{\sim}{X}, \underset{\sim}{\lambda}^{(k)}, S)$ for an estimate $\underset{\sim}{\lambda}^{(k)}$ of $\underset{\sim}{\lambda}^*$ is the inner iteration. Let $\underset{\sim}{X}^{(k)} = X(\underset{\sim}{\lambda}^{(k)}, S)$ be an unconstrained minimizer of $T(\underset{\sim}{X}, \underset{\sim}{\lambda}^{(k)}, S)$. In the outer iteration the estimate $\underset{\sim}{\lambda}^{(k)}$ is updated so as to cause $\underset{\sim}{X}^{(k)} \to \underset{\sim}{X}^*$. Hestenes suggested the following formula for adjusting the multiplier vector $\underset{\sim}{\lambda}^{(k)}$

$$\underset{\sim}{\lambda}^{(k+1)} = \underset{\sim}{\lambda}^{(k)} - S^{(k)} \; \underset{\sim}{C}(\underset{\sim}{X}^{(k)}) \qquad [15]$$

where $S^{(k)} = \sigma^{(k)} I$, $0 < \sigma^{(k)} \leqq \sigma$, $\sigma^{(k)} = \gamma\sigma$ and $0 < \gamma \leqq 1$. The relation [15] is derived from the observation that $\underset{\sim}{X}^{(k)}$ is a local minimizer of $T(\underset{\sim}{X}, \underset{\sim}{\lambda}^{(k)}, S)$ and $\underset{\sim}{\lambda}^{(k+1)}$ is chosen so that first order necessary conditions are satisfied at $\underset{\sim}{X}^{(k)}$ for P2. Hestenes (H2) did not analyze the convergence of the method, but subsequently (H4) established that the method converges linearly and superlinear convergence may be achieved when $\sigma \to \infty$. In practical applications very fast linear convergence occurs for a large but finite value of σ. Convergence is induced by not only a large value of σ but also by multiplier iteration [15] (F8).

In Powell's method when S is fixed and $\underset{\sim}{\theta}$ parameters are adjusted to let $\underset{\sim}{X}^{(k)} \to \underset{\sim}{X}^*$, the unique Lagrange multiplier vector $\underset{\sim}{\lambda}^* = S \; \underset{\sim}{\theta}^*$, where $\underset{\sim}{\theta}^*$

corresponds to the vector of parameters at $\underset{\sim}{X}^*$. This implies that a connection can be established between the augmented function ϕ in [8] and T in [14] using the relationship

$$\lambda_i = \sigma_i \theta_i, \quad i = 1, 2, \ldots, m. \qquad [16]$$

From [8], [14] and [16],

$$\phi(\underset{\sim}{X}, \underset{\sim}{\theta}, S) = T(\underset{\sim}{X}, \underset{\sim}{\lambda}, S) + \frac{1}{2} \sum_{i=1}^{m} \lambda^2{}_i/\sigma_i. \qquad [17]$$

The difference between ϕ and T is independent of $\underset{\sim}{X}$. If $\underset{\sim}{X}(\underset{\sim}{\theta}, S)$ and $\underset{\sim}{X}(\underset{\sim}{\lambda}, S)$ are unconstrained minimizers of ϕ and T respectively for any S and if $\underset{\sim}{\theta}$ and $\underset{\sim}{\lambda}$ are related as in [16], then $\underset{\sim}{X}(\underset{\sim}{\theta}, S) = \underset{\sim}{X}(\underset{\sim}{\lambda}, S)$. Therefore the iterative methods suggested by Powell and Hestenes for changing $\underset{\sim}{\theta}$ and $\underset{\sim}{\lambda}$ parameters are the same.

In view of the equivalence relationship [17] between ϕ and T, the numerical algorithm A1 is discussed in terms of the augmented penalty function T. In the outer iteration adjustment of $\underset{\sim}{\lambda}$ parameters using [15] is considered, assuming that $\underset{\sim}{\theta}$ and $\underset{\sim}{\lambda}$ are related by [16]. The algorithm A1 is discussed and analyzed using $\underset{\sim}{\lambda}$ parameters to emphasize the primal-dual nature of the method which iterates with an approximation $\underset{\sim}{\lambda}^{(k)}$ to the Lagrange multipliers λ^* in such a way as to make $\underset{\sim}{\lambda}^{(k)} \rightarrow \underset{\sim}{\lambda}^*$.

The algorithm A1 is now modified and denoted as the Powell-Hestenes augmented penalty function algorithm A2. The convergence of the algorithm is measured in terms of $B = \max_i |c_i(\underset{\sim}{X})|$.

Algorithm A2:

```
(i)   Select $\underset{\sim}{\lambda}^{(1)} = \underset{\sim}{\lambda}^{(0)}$, $S^{(1)} = S^{(0)}$, $k = 0$, arbitrary starting
      point $\underset{\sim}{X}^{(0)}$ and $B^{(1)} = B_0$ where $B_0 \geqq \max_i |c_i(\underset{\sim}{X}^{(0)})|$.
(ii)  $k = k + 1$
(iii) Minimize $T(\underset{\sim}{X}, \underset{\sim}{\lambda}^{(k)}, S^{(k)})$ to find $\underset{\sim}{X}^{(k)} = \underset{\sim}{X}(\underset{\sim}{\lambda}^{(k)}, S^{(k)})$
      starting the unconstrained minimization from $\underset{\sim}{X}^{(k-1)}$.
(iv)  Find $\mathcal{D} = \{i: \ |c_i(\underset{\sim}{X}^{(k)})| \geqq B^{(k)}/4\}$.
      If $\max_i |c_i(\underset{\sim}{X}^{(k)})| \geqq B^{(k)}$, set $B^{(k+1)} = B^{(k)}$. Go to (vii).
(v)   $B^{(k+1)} = \max_i |c_i(\underset{\sim}{X}^{(k)})|$. If $B^{(k+1)} \leqq \mathcal{E}$ stop. The $\mathcal{E}$ is a
      specified tolerance for B.
(vi)  If $B^{(k+1)} \leqq B^{(k)}/4$ or $\underset{\sim}{\lambda}^{(k)} = \underset{\sim}{\lambda}^{(k-1)}$
      set $\underset{\sim}{\lambda}^{(k+1)} = \underset{\sim}{\lambda}^{(k)} - S^{(k)} \underset{\sim}{C}(\underset{\sim}{X}^{(k)})$
      $S^{(k+1)} = S^{(k)}$, go to (ii).
(vii) Set $\underset{\sim}{\lambda}^{(k+1)} = \underset{\sim}{\lambda}^{(k)}$
        $\sigma_i^{(k+1)} = 10\, \sigma_i^{(k)} \quad \forall i \in \mathcal{D}$,
      go to (ii).
```

When second order sufficiency conditions hold good at $\underset{\sim}{X}^*$ for P2, there exists a $\sigma' > 0$ such that for $\sigma_i \geqq \sigma'$ $\forall i$, the Hessian matrix of both $\phi(\underset{\sim}{X}, \underset{\sim}{\theta}^*, S)$ and $T(\underset{\sim}{X}, \underset{\sim}{\lambda}^*, S)$ at $\underset{\sim}{X}^*$ is positive definite and $\underset{\sim}{X}^*$ is a strong local minimum of $\phi(\underset{\sim}{X}, \theta^*, S)$ and $T(\underset{\sim}{X}, \underset{\sim}{\lambda}^*, S)$ (B2), (B7), (F8), (H2). It should be noted that the local convexity of $\phi(\underset{\sim}{X}, \underset{\sim}{\theta}^*, S)$ and $T(\underset{\sim}{X}, \underset{\sim}{\lambda}^*, S)$ near $\underset{\sim}{X}^*$ is established without any assumptions about the convexity of problem P2. The aim of the algorithm A2 is to keep S constant and adjust $\underset{\sim}{\lambda}^{(k)}$ so as to cause $\underset{\sim}{\lambda}^{(k)} \rightarrow \underset{\sim}{\lambda}^*$.

Therefore in subsequent discussions it is assumed that $\sigma_i \geq \sigma' \; \forall i$ have been chosen and held fast so that ϕ and T are locally convex. Due to this reason the explicit dependence of $\underset{\sim}{X}$ on S is dropped and $\underset{\sim}{X}(\underset{\sim}{\lambda}, S)$ is represented as $\underset{\sim}{X}(\underset{\sim}{\lambda})$.

Haarhoff and Buys (H1) proposed a numerical algorithm very similar to the Powell-Hestenes method. They were motivated by the following observations about the traditional quadratic penalty function approach to solve P2. Let the quadratic penalty function for P2 be

$$P(\underset{\sim}{X}, \sigma) = f(\underset{\sim}{X}) + \sigma \sum_{i=1}^{m} (c_i(\underset{\sim}{X}))^2, \quad \sigma > 0.$$

Let $\underset{\sim}{X}(\sigma)$ be an unconstrained minimizer of $P(\underset{\sim}{X}, \sigma)$ for a large value of control parameter σ and $\underset{\sim}{X}^*$ be a local minimizer of P2. The gradient of $P(\underset{\sim}{X}, \sigma)$ is zero at $\underset{\sim}{X}(\sigma)$ but the gradient at $\underset{\sim}{X}^*$ is $\underset{\sim}{\nabla} f(\underset{\sim}{X}^*)$. Therefore, in the usual case when $\underset{\sim}{\nabla} f(\underset{\sim}{X}^*)$ is nonzero, $\underset{\sim}{X}(\sigma)$ and $\underset{\sim}{X}^*$ have to be different. Let $\hat{\underset{\sim}{X}}$ be a solution to the under-determined system of equations $\underset{\sim}{C}(\underset{\sim}{X}) = 0$. At $\hat{\underset{\sim}{X}}$ the gradient of $P(\underset{\sim}{X}, \sigma)$ is $\underset{\sim}{\nabla} f(\hat{\underset{\sim}{X}})$ which is generally not zero. Therefore $\hat{\underset{\sim}{X}}$ and $\underset{\sim}{X}(\sigma)$ are different and for any finite value of σ, $\underset{\sim}{X}(\sigma)$ is neither a solution to P2 nor satisfies $\underset{\sim}{C}(\underset{\sim}{X}) = 0$. Usually $\underset{\sim}{X}(\sigma)$ tends to $\underset{\sim}{X}^*$ when $\sigma \to \infty$ (L5), (Z1). From these observations Haarhoff and Buys added a linear combination of constraints to $P(\underset{\sim}{X}, \sigma)$ to obtain

$$T(\underset{\sim}{X}, \underset{\sim}{\lambda}, S) = f(\underset{\sim}{X}) - \underset{\sim}{\lambda}^T \underset{\sim}{C}(\underset{\sim}{X}) + \frac{1}{2} (\underset{\sim}{C}(\underset{\sim}{X}))^T S\underset{\sim}{C}(\underset{\sim}{X}), \quad S = \sigma I$$

where $\underset{\sim}{\lambda} \varepsilon E^m$ and $\sigma > 0$. This function achieved their objective, i.e., balanced the gradient of $f(\underset{\sim}{X})$ in the vicinity of the minimum by a linear combination of gradients of constraint functions $\underset{\sim}{C}(\underset{\sim}{X})$.

The augmented penalty function proposed by Haarhoff and Buys is identical to the Powell-Hestenes augmented penalty function for P2. However the numerical algorithm of Haarhoff and Buys has some distinct features. They noted that the multiplier updates [15] are valid only when the function $T(\underset{\sim}{X}, \underset{\sim}{\lambda}^{(k)}, S)$ is minimized exactly for each $\underset{\sim}{\lambda}^{(k)}$ and that it is better to terminate the inner iterations when a better value of $T(\underset{\sim}{X}, \underset{\sim}{\lambda}^{(k)}, S)$ is obtained. They suggested that the multipliers in the outer iteration be obtained from the first order necessary condition.

$$\underset{\sim}{\nabla} f(\underset{\sim}{X}^{(k)}) = N(\underset{\sim}{X}^{(k)})\ \underset{\sim}{\lambda}, \quad \underset{\sim}{\lambda} \in E^m. \qquad [18]$$

The condition [18] represents an over-determined system of n equations in m parameters. Taking the scalar product of [18] with each $\underset{\sim}{\nabla} C_i(\underset{\sim}{X}^{(k)})$, the following system of equations is obtained.

$$N^T(\underset{\sim}{X}^{(k)})\ \underset{\sim}{\nabla} f(\underset{\sim}{X}^{(k)}) = N^T(\underset{\sim}{X}^{(k)})\ N(\underset{\sim}{X}^{(k)})\ \underset{\sim}{\lambda}, \quad \underset{\sim}{\lambda} \in E^m. \qquad [19]$$

The expression in [19] represents a system of m equations in m parameters $\underset{\sim}{\lambda}$ that may easily be solved for $\underset{\sim}{\lambda}$. This, in effect, is a least squares' solution to [18]. The vector of multipliers $\underset{\sim}{\lambda}$ is an estimate of the unique Lagrange multiplier vector $\underset{\sim}{\lambda}^*$ at $\underset{\sim}{X}^*$ and $\underset{\sim}{\lambda}$ tends to $\underset{\sim}{\lambda}^*$.

Haarhoff and Buys were more concerned with computational considerations than with convergence or duality aspects of the algorithm. They suggested that the problem functions be scaled so that the gradients are of the same magnitude and σ_i be on the order of ten. In this algorithm σ_i $i = 1, 2, \ldots, m$ are kept constant and in the inner iteration the variable metric method of

Davidon-Fletcher-Powell (DFP) is used to minimize $T(\underset{\sim}{X}, \underset{\sim}{\lambda}^{(k)}, S)$. The approximation to $[\nabla^2 T]^{-1}$ is updated using the DFP update formula (M11). A restoration step is included in the inner iteration and in this step T is minimized without using derivatives in a direction that leads to the satisfaction of linearized constraints. Other numerical aspects of the algorithm, such as the various stopping criteria for inner and outer iterations and updating the approximation to inverse Hessian $[\nabla^2 T]^{-1}$ are discussed in reference (H1).

The elegant idea of local convexification of the Lagrangian was first introduced by Arrow and Solow (A1). They suggested addition of quadratic penalty terms to the classical Lagrangian to arrive at a modified Lagrangian that was locally convex. They were motivated by adaptation of the differential gradient scheme, developed by Arrow, et al. (A1) for approaching saddle points of convex programs, to nonconvex programs. Their differential gradient method is a small step-size algorithm while those of Hestenes, Powell and Haarhoff and Buys are large step-size methods.

In the above contributions to the augmented penalty function technique duality concepts were not employed. Primal-dual interpretation of the technique was analyzed by Buys (B7), Luenberger (L5), Rockafellar (R12) and Bertsekas (B2), (B3). A detailed review of the duality results may be found in reference (F8). The duality results are summarized briefly in the next section.

3.3 Review of the Technique for a Constrained Problem with Equalities and Inequalities

3.3.1 Constrained Problem

The problem P3 with equality and inequality constraints is represented as

$$\text{P3:}\quad \text{Minimize } f(\underset{\sim}{X}),\quad \underset{\sim}{X} \in \mathcal{L} \subseteq \mathcal{E}^n$$

$$\text{Subject to } c_i(\underset{\sim}{X}) = 0 \quad i = 1, 2, \ldots, k$$

$$c_i(\underset{\sim}{X}) \geqq 0 \quad i = k+1, \ldots, m, \quad 0 \leqq k \leqq n.$$

The real valued functions $f(\underset{\sim}{X})$ and $c_i(\underset{\sim}{X})$ $\forall i$ are defined on a nonempty open set $\mathcal{L} \subseteq \mathcal{E}^n$. Let $\underset{\sim}{X}^*$ be a local optimal solution to P3. The problem functions are of class $C^{(2)}$ on $\mathcal{L}$ and specifically in an open neighborhood of $\underset{\sim}{X}^*$. The Lagrangian associated with P3 is

$$L(\underset{\sim}{X}, \underset{\sim}{\lambda}) = f(\underset{\sim}{X}) - \underset{\sim}{\lambda}^T \underset{\sim}{C}(\underset{\sim}{X}), \quad \underset{\sim}{\lambda} \in \mathcal{E}^m, \quad \underset{\sim}{X} \in \mathcal{L} \subseteq \mathcal{E}^n. \qquad [20]$$

The following conditions are assumed to hold good at $\underset{\sim}{X}^*$ (F1), (M13).

(1) $\underset{\sim}{X}^*$ is a regular point of the feasible region

$\mathcal{F} = \{\underset{\sim}{X}: \; C_i(\underset{\sim}{X}) = 0, \; 1 \leqq i \leqq k \text{ and } C_i(\underset{\sim}{X}) \geqq 0, \; k < i \leqq m\}$

Let $E = \{i: \; 1 \leqq i \leqq k\}$

$I = \{i: \; C_i(\underset{\sim}{X}^*) = 0, \; k < i \leqq m\}$. The $\underset{\sim}{X}^*$ is a regular point of $\mathcal{F}$ when $\{\underset{\sim}{\nabla} C_i(\underset{\sim}{X}^*)\}$ $i \in E \subseteq I$ is a linearly independent set.

(2) There exists an unique Lagrange multiplier vector $\underset{\sim}{\lambda}^* \in \mathcal{E}^m$ such that the Kuhn-Tucker conditions are satisfied at $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$

$$C_i(\underset{\sim}{X}^*) = 0 \quad i \in E$$

$$C_i(\underset{\sim}{X}^*) \geqq 0 \quad \lambda_i^* \geqq 0, \quad \lambda_i^* \, C_i(\underset{\sim}{X}^*) = 0 \quad i \notin e \qquad [21]$$

$$\underset{\sim}{\nabla} L(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*) = 0$$

These are first-order necessary conditions for local optimality at $\underset{\sim}{X}^*$ and $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*) \in \mathcal{E}^{n+m}$ satisfying [21] is termed a Kuhn-Tucker point.

(3) Second-order necessary conditions for local optimality of $\underset{\sim}{X}^*$ are that in addition to [21]

$$\underset{\sim}{Y}^T \nabla^2 L(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*) \underset{\sim}{Y} \geqq 0 \quad \forall \underset{\sim}{Y} \in \mathcal{Y}^* \subseteq \mathcal{E}^n \qquad [22]$$

where

$$\mathcal{Y}^* = \{\underset{\sim}{Y}: \ \underset{\sim}{Y}^T \underset{\sim}{\nabla C}_i(\underset{\sim}{X}^*) = 0, \ \ i \in E \subseteq I^* \text{ and}$$

$$\underset{\sim}{Y}^T \underset{\sim}{\nabla C}_i(\underset{\sim}{X}^*) \geqq 0, \ \ i \in I - I^*\},$$

I is the index set of active inequalities, I* is the index set of strongly active inequalities and I - I* is the index set of weakley active constraints. However the following weaker second-order necessary condition is usually assumed instead of [22] (F1), (M11).

$$\underset{\sim}{Y}^T \nabla^2 L(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*) \underset{\sim}{Y} \geqq 0 \quad \forall \underset{\sim}{Y} \in \mathcal{Y} \subseteq \mathcal{E}^n \qquad [23]$$

$$\mathcal{Y} = \{\underset{\sim}{Y}: \ \underset{\sim}{Y}^T \underset{\sim}{\nabla C}_i(\underset{\sim}{X}^*) = 0, \ \ i \in E \subseteq I\}.$$

(4) Strict complementarity holds at $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ when

$$\lambda_i^* \neq 0 \text{ for each } 1 \leqq i \leqq m \text{ for which } C_i(\underset{\sim}{X}^*) = 0. \qquad [24]$$

A weaker form of [24] is

$$\lambda_i^* > 0 \text{ and } C_i(\underset{\sim}{X}^*) = 0, \ \ i \in I. \qquad [25]$$

(5) Second-order sufficient conditions for $\underset{\sim}{X}^*$ to be an isolated local minimum are that in addition to [21] and [23]

$$\underset{\sim}{Y}^T \underset{\sim}{\nabla}^2 (\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*) \underset{\sim}{Y} > 0 \quad \forall \text{ nonzero } \underset{\sim}{Y} \in \mathcal{Y}^*. \qquad [26]$$

However the condition [26] is usually replaced by the verifiable condition (M11),

$$\underset{\sim}{Y}^T \nabla^2 L(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)\, \underset{\sim}{Y} > 0 \quad \forall \text{ nonzero } \underset{\sim}{Y} \in \mathcal{Y}. \qquad [27]$$

3.3.2 Powell - Hestenes - Rockafellar Penalty Function

The augmented Lagrangian penalty function for P3 is obtained by combining the Powell-Hestenes penalty function T and the Rockafellar penalty function T. The combined function may be represented as

$$T_{PHR}(\underset{\sim}{X}, \underset{\sim}{\lambda}, \underset{\sim}{\sigma}) = f(\underset{\sim}{X}) - \sum_{i\varepsilon E} [\lambda_i\, C_i(\underset{\sim}{X}) - \frac{1}{2}\sigma_i\, C_i^{\,2}(\underset{\sim}{X})] + \frac{1}{2} \sum_{i\varepsilon E} [\sigma_i (C_i(\underset{\sim}{X}) - \frac{\lambda_i}{\sigma_i})^2 - \lambda_i^{\,2}/\sigma_i] \qquad [28]$$

where

$$(C_i(\underset{\sim}{X}) - \frac{\lambda_i}{\sigma_i}) = \min\, [(C_i(\underset{\sim}{X}) - \frac{\lambda_i}{\sigma_i}),\ 0]$$

$$\underset{\sim}{\sigma} \in \mathcal{E}^m_{++}, \quad \underset{\sim}{\lambda} \in \mathcal{E}^m.$$

In [28], the factor λ_i/σ_i represents a penalizing threshold for the ith inequality constraint. The multipliers λ_i $\forall i$ are unconstrained and this is an useful property of the augmented penalty function T_{PHR}. Further the function T_{PHR} possesses a number of strong properties not exhibited by the classical Lagrangian $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$. The following properties of T_{PHR} make it ideal for use in a primal-dual algorithm for solving P3.

Let $M(\underset{\sim}{\lambda})$ be the index set of the inequalities that contribute to the quadratic penalty term in T_{PHR} for an estimate, $\underset{\sim}{\lambda}$, of the Lagrange multiplier vector $\underset{\sim}{\lambda}^*$.

$$M(\underset{\sim}{\lambda}) = \{i:\ i \notin E,\ \ C_i(\underset{\sim}{X}) < \lambda_i/\sigma i\}. \qquad [29]$$

Equivalently,

$$M(\underset{\sim}{\lambda}) = \{i:\ i \notin E,\ \lambda_i - \sigma_i\ C_i(\underset{\sim}{X}) > 0\}. \qquad [30]$$

At the local optimum $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ of P3, $M(\underset{\sim}{\lambda}^*)$ is the index set, I*, of the strongly active inequalities. By the strict complementarity assumption, I = I* and therefore $M(\underset{\sim}{\lambda}^*)$ represents the active inequality constraints at the local optimum $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$. Further the set $\overline{E \cup M(\underset{\sim}{\lambda})}$ represents the inactive inequality constraints at the intermediate approximation $(\underset{\sim}{X}, \underset{\sim}{\lambda})$ to the solution $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$. Let $L = \overline{E \cup M(\underset{\sim}{\lambda})}$. Then,

$$L = \{i:\ i \notin E,\ \ C_i(\underset{\sim}{X}) \geqq \lambda_i/\sigma_i\}. \qquad [31]$$

Equivalently,

$$L = \{i:\ i \notin E,\ \ \underset{\sim}{\lambda}_i - \sigma_i\ C_i(\underset{\sim}{X}) \geqq 0\}. \qquad [32]$$

Using the above results the augmented penalty function T_{PHR} may be represented as follows.

$$T_{PHR}\ (\underset{\sim}{X}, \underset{\sim}{\lambda}, \underset{\sim}{\sigma}) = f(\underset{\sim}{X}) - \sum_{i \in E\ M(\underset{\sim}{\lambda})} (\lambda_i - \frac{1}{2}\sigma_i\ C_i(\underset{\sim}{X}))\ C_i(\underset{\sim}{X})$$

$$- \frac{1}{2} \sum_{i \in L} \lambda_i^{\ 2}/\sigma_i. \qquad [33]$$

The representation of T_{PHR} in [33] clearly illustrates that it is obtained by combining the Powell-Hestenes penalty function T and the Rockafellar penalty function T.

Mangasarian (M2) associated a wide class of Lagrangians with the nonconvex program P3. The unconstrained stationary points and local saddle-points of each Lagrangian were shown to be related to the Kuhn-Tucker points or local or global solutions of P3 (M2). The Lagrangians considered by Mangasarian (M2) were twice differentiable globally. The augmented penalty function T_{PHR} belongs to the general class of Lagrangians investigated by Mangasarian (M2). However the penalty function T_{PHR} is twice continuously differentiable in $\underset{\sim}{X}$ except at points where $\lambda_i - \sigma_i \, c_i(\underset{\sim}{X}) = 0, \quad i \in M(\underset{\sim}{\lambda})$. By the strict complementarity condition, $\lambda_i - \sigma_i \, c_i(\underset{\sim}{X}^*) \neq 0$ for $i \in M(\underset{\sim}{\lambda}^*)$, i.e., $i \in I$. Therfore T_{PHR} is twice continuously differentiable in an open neighborhood about $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$.

Mangasarian (M2) established the properties of the general class of Lagrangians for P3. As T_{PHR} is a member of this class of Lagrangians, the following properties hold good for T_{PHR} (M2). These properties of T_{PHR} also were established by Rockafellar (R6). For $\underset{\sim}{\sigma} \in E^m_{++}$, $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ is a Kuhn-Tucker point of P3 if and only if it is a stationary point of T_{PHR}. For large but finite σ_i, $\nabla^2 T_{PHR}$ is positive definite (M2), (A3) and

$$T_{PHR}\,(\underset{\sim}{X}^*, \underset{\sim}{\lambda}, \underset{\sim}{\sigma}) \leqq T_{PHR}\,(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*, \underset{\sim}{\sigma}) \leqq T_{PHR}\,(\underset{\sim}{X}, \underset{\sim}{\lambda}^*, \sigma) \qquad [34]$$

$\forall\ \underset{\sim}{\lambda} \in E^m$, $\underset{\sim}{X} \in A$ where A is some open neighborhood of $\underset{\sim}{X}^*$. Conversely, if $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ is a saddle-point satisfying [34], then $\underset{\sim}{X}^*$ is a solution of P3 for $\underset{\sim}{X} \in A$.

A duality theory in terms of extended Lagrangians was presented by Mangasarian (M2). The augmented dual problem may be represented as

D3: Maximize $g(\underset{\sim}{\lambda}, \underset{\sim}{\sigma})$.

$$g(\underset{\sim}{\lambda}, \underset{\sim}{\sigma}) = \inf_{\underset{\sim}{X} \varepsilon L} T_{PHR} (\underset{\sim}{X}, \underset{\sim}{\lambda}, \sigma) \qquad [35]$$

The augmented dual function $g(\underset{\sim}{\lambda}, \underset{\sim}{\sigma})$ is concave in $(\underset{\sim}{\lambda}, \underset{\sim}{\sigma})$ and is strictly nondecreasing in $\underset{\sim}{\sigma}$. If the point $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ satisfies the optimality conditions and if $\underset{\sim}{\sigma}$ is sufficiently large, then $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ is an isolated local maximum of D3. Conversely, if $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ is a global or local solution of D3, then the optimality conditions for P3 are satisfied at $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$

Let $\underset{\sim}{X}(\underset{\sim}{\lambda}) = \underset{\sim}{X}(\underset{\sim}{\lambda}, \underset{\sim}{\sigma})$ be an unconstrained minimizer of $T_{PHR} (\underset{\sim}{X}, \underset{\sim}{\lambda}, \underset{\sim}{\sigma})$ for $\underset{\sim}{\lambda}$ in an open neighborhood of $\underset{\sim}{\lambda}^*$. Then the dual function at this point may be expressed as

$$g(\underset{\sim}{\lambda}, \underset{\sim}{\sigma}) = T_{PHR} (\underset{\sim}{X} (\underset{\sim}{\lambda}), \underset{\sim}{\lambda}, \underset{\sim}{\sigma}) = T_{PHR} (\underset{\sim}{\lambda}). \qquad [36]$$

Useful duality results for multiplier iterations may be summarized as follows (F8).

$$\frac{\partial T_{PHR}(\underset{\sim}{\lambda})}{\partial \lambda_i} = \begin{cases} -C_i(\underset{\sim}{X}(\underset{\sim}{\lambda})) & i \varepsilon E \\ -\min(C_i(\underset{\sim}{X} (\underset{\sim}{\lambda})), \lambda_i/\sigma_i) & i \notin E \end{cases} \qquad [37]$$

Let N be a matrix with $\nabla \underset{\sim}{c}_i(\underset{\sim}{X})$, $i \varepsilon E \cup M(\underset{\sim}{\lambda})$ as columns and G be the Hessian of T_{PHR}. Then

$$\nabla^2_{\underset{\sim}{\lambda}} T_{PHR} = \begin{array}{|c|c|l} \hline -N^T G^{-1} N & 0 & \quad i \varepsilon E \cup M(\underset{\sim}{\lambda}) \\ \hline 0 & -S^{-1} & \quad i \varepsilon E \cup M(\underset{\sim}{\lambda}) \\ \hline \end{array} \qquad [38]$$

Because $\underset{\sim}{X}^* = \underset{\sim}{X}(\lambda^*, \underset{\sim}{\sigma})$ for large $\underset{\sim}{\sigma}$, the optimality conditions and the expressions [37] and [38] imply that T_{PHR} is concave in $\underset{\sim}{\lambda}$ for $\underset{\sim}{\lambda}$ close to $\underset{\sim}{\lambda}^*$ is a strong unconstrained maximizer of T_{PHR}.

The above results indicate that the problem P3 may be solved by locating a saddle-point of T_{PHR}. The saddle-point theory and local duality results suggest a primal-dual algorithm for solving P3. The algorithm consists of inner and outer iterations and is similar to the algorithm A2. In the inner iteration, k, for fixed $\underset{\sim}{\lambda}^{(k)}$ and $\underset{\sim}{\sigma}^{(k)}$, T_{PHR} $(\underset{\sim}{X}, \underset{\sim}{\lambda}^{(k)}, \underset{\sim}{\sigma}^{(k)})$ is minimized with respect to $\underset{\sim}{X}$ starting the unconstrained minimization from $\underset{\sim}{X}^{(k-1)}$. The initial starting point $\underset{\sim}{X}^{(0)}$ need not be feasible and may be chosen arbitrarily. Let $\underset{\sim}{X}^{(k)} = \underset{\sim}{X}(\underset{\sim}{\lambda}^{(k)}, \underset{\sim}{\sigma}^{(k)})$ be the unconstrained minimizer of T_{PHR} $(\underset{\sim}{X}, \underset{\sim}{\lambda}^{(k)}, \underset{\sim}{\sigma}^{(k)})$. In the outer iteration $\underset{\sim}{\sigma}^{(k)}$ is increased so as to force $(\underset{\sim}{X}^{(k)}, \underset{\sim}{\lambda}^{(k)})$ into a region about $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ and $\underset{\sim}{\lambda}^{(k)}$ is adjusted so as to ensure $\underset{\sim}{\lambda}^{(k)} \rightarrow \underset{\sim}{\lambda}^*$ and $\underset{\sim}{X}^{(k)} \rightarrow \underset{\sim}{X}^*$.

The duality relationships [37] and [38] suggest gradient and Newton steps for adjusting $\underset{\sim}{\lambda}$ in the outer iteration so as to maximize the dual function. Mangasarian (M2) analyzed the method of multipliers with a gradient step for adjusting $\underset{\sim}{\lambda}$ in the outer iteration.

$$\underset{\sim}{\lambda}^{(k+1)} = \underset{\sim}{\lambda}^{(k)} + \beta \underset{\sim\sim}{\nabla\lambda}\, T_{PHR}\ (\underset{\sim}{\lambda}). \qquad [39]$$

He established the linear convergence of this algorithm with exact minimizations in the inner iteration and a large but finite $\underset{\sim}{\sigma}$. He also investigated the relation between β and the speed of convergence of the method.

The convergence and duality analyses presented by Rockafellar (R6) also are valid for the primal-dual algorithm for P3. Rockafellar (R6) established the convergence of the algorithm with inexact minimizations in the inner iteration. Pierre and Lowe (P2) comprehensively reviewed the technique for P3 and presented a numerical algorithm, test problems and computational results. In this implementation of the ALAG penalty function technique in a numerical algorithm, a simple gradient step for adjusting $\underset{\sim}{\lambda}$ was used in the outer iteration.

$$\underset{\sim}{\lambda}^{(k+1)} = \underset{\sim}{\lambda}^{(k)} + S\nabla\underset{\sim}{\lambda}\ T_{PHR}\ (\underset{\sim}{\lambda}). \qquad [40]$$

The penalty parameters σ_i were monotonically increased in the outer iteration. The linear constraints were also included in the penalty term. A constraint with upper and lower bounds was treated as two separate constraints. This approach introduces two dual variables for such a constraint.

Fletcher (F8) suggested second-order $\underset{\sim}{\lambda}$ iteration updates. He also devised a Newton-like iteration for updating $\underset{\sim}{\lambda}$ using estimates of G in [38]. In the numerical experiments, Fletcher (F8) used a quasi-Newton method for unconstrained minimization of T_{PHR} and built-up estimate of G. The change in G was accounted for when $\underset{\sim}{\sigma}$ was changed. The computational results presented by Fletcher (F8) indicate that the Newton-like algorithm for updating $\underset{\sim}{\lambda}$ is more efficient that the gradient step for adjusting $\underset{\sim}{\lambda}$. In these numerical experiments the penalty constants σ_i were also adjusted (F8). Fletcher (F8) showed that this scheme for adjusting σ_i never fails to induce convergence of the algorithm and avoids increasing σ_i by an arbitrary factor of 10.

Buys and Gonin (B9) performed sensitivity analysis with the aid of the ALAG penalty function T_{PHR}. Similar sensitivity results were developed by Armacost and Fiacco (A3) using augmented Lagrangian function T_{PHR}. In these analyses the following parametric mathematical programming problem was considered.

$$\begin{aligned} P\dot{3}(\underset{\sim}{a})\text{:}\quad & \text{Minimize}\quad f(\underset{\sim}{X}, \underset{\sim}{a}),\ \underset{\sim}{X} \varepsilon E^{n},\ \ \underset{\sim}{a} \varepsilon E^{v} \qquad [41] \\ & \text{Subject to } c_i(\underset{\sim}{X}, \underset{\sim}{a}) = 0,\ i = 1, 2, \ldots, k \\ & \qquad\qquad\quad c_i(\underset{\sim}{X}, \underset{\sim}{a}) \geqq 0,\ i = k+1, k+2, \ldots, m \\ & \qquad\qquad\quad 0 \leqq k \leqq n \end{aligned}$$

In [41] $\underset{\sim}{a}$ is the vector of sensitivity parameters. In these analyses, the problem functions were assumed to be twice continuously differentiable in $(\underset{\sim}{X}, \underset{\sim}{a})$ in a neighborhood of $(\underset{\sim}{X}*, \underset{\sim}{a}*)$ and for some $\underset{\sim}{a}*$, the conditions in 3.4.1 were assumed to hold at $(\underset{\sim}{X}*, \underset{\sim}{a}*, \underset{\sim}{\lambda}*)$. The $\underset{\sim}{\lambda}*$ is the vector of Lagrange multipliers associated with a solution $\underset{\sim}{X}*$ to P3 $(\underset{\sim}{a}*)$.

IV. NUMERICAL RESULTS

4.1 Introduction

Numerical experiments have been conducted to identify the most efficient ALAG Penalty Function Technique for computer implementation. These numerical exercises, include testing individual unconstrained optimizers and constrained optimizers utilizing a wide range of inequality and equality constrained nonlinear optimization problems. Phase one of these numerical experiments involved testing a number of popular unconstrained optimization algorithms. The most effective of these algorithms were then incorporated into ALAG Penalty Function routines for the solution of constrained optimization problems.

4.2 Unconstrained Optimizing Algorithms

Two different classes of algorithms for solving the unconstrained optimization problems have been tested on several sample problems. The first class of algorithms tested were those that do not require derivative functions. These algorithms make use of finite difference approximations for derivatives or work solely with the given problem function in seeking an optimum. The second class of unconstrained optimizers require explicit first derivative functions. The unconstrained optimization techniques are identified in the following table and discussed in (L5).

These algorithms performance on a number of sample problems is described in Table II. Based on the results presented in Table II and computer programming considerations algorithms 4, 5 and 7 were incorporated into computerized ALAG Penalty Function routines and tested with a number

TABLE I

UNCONSTRAINED OPTIMIZERS TESTED

Derivative Free Optimizers

1. Hooke-Jeeves Pattern Search Algorithm
2. Powell's Algorithm
3. Stewarts Adaptation of the Davidon-Fletcher-Powell Algorithm
4. Fletcher's Finite Difference Technique for a Complimentary Davidon-Fletcher-Powell Algorithm

First Derivatives Required

5. Complimentary Davidon-Fletcher-Powell Algorithm
6. Davidon's Variance Algorithm
7. Complimentary Davidon-Fletcher-Powell Algorithm (with no line searches)

TABLE II

NUMBER OF FUNCTION EVALUATIONS FOR THE UNCONSTRAINED OPTIMIZERS

	Unconstrained Optimizer						
Problem	1	2	3	4	5	6	7
1. $F(X) = 100(X_2-X_1^2)^2 + (1-X_1)^2 + 0.5(202X_1X_2-1)^2 + 1818(X_2^2+X_1)^2$	111	62	110	75	15	16	43
2. $F(X) = 0.01X_1^2 + X_2^2 + 0.00916(X_1X_2-36.1483)^2$	117	42	37	48	10	13	13
3. $F(X) = 100(X_2-X_1^2)^2 + (1-X_1)^2 + 1548.34(4.91667-X_1)^2 + 7812.92(X_1^2+X_2^2-1.0106)^2$	140	42	37	38	9	8	13
4. $F(X) = X_1^2 + X_2^2 + X_3^2 + 4.009(X_1^2+X_2^2-1.0124)^2$	130	30	27	44	8	*	43
5. $F(X) = (X_1-10)^3 + (X_2-20)^3 + 4(X_1-13)^2 + 0.00059(6-X_1)^2 - (X_2+25)$	254	*	138	153	24	38	82
6. $F(X) = X_1X_2X_3 + (X_1+2X_2+2X_3)^2$	239	*	128	*	*	19	37
7. $F(X) = 100(X_2-X_1^3) + (1-X_1)^2$	452	143	91	169	58	26	58
8. $F(X) = (1.5-X_1(1-X_2))^2 + (2.25-X_1(1-X_2^2))^2 + (2.625-X_1(1-X_2^3))^2$	266	49	*	53	16	18	22
9. $F(X) = (X_1+10X_2)^2 + 5(X_3-X_4)^2 + (X_2-2X_3)^4 + 10(X_1-X_4)^4$	791	190	*	322	67	26	55
10. $F(X) = (e^{X_1}-X_2)^4 + 100(X_2-X_3)^6 + (\tan(X_3-X_4))^4 + X_1^8 + (X_4-1)^2$	234	280	99	999	105	27	94

*Didn't converge to an optimum point.

of inequality and equality constrained nonlinear optimization problems.

4.3 ALAG Constrained Optimizing Algorithms

The selected ALAG routines were tested on many of the example constrained problems presented in (B6). Table III summarizes the computational results achieved for these example problems where the algorithrms tested were

1. ALAG algorithm with unconstrained optimizer 5 (see Table I).
2. ALAG algorithm with unconstrained optimizer 7 (see Table I).
3. ALAG algorithm with unconstrained optimizer 4 (see Table I).

TABLE III

COMPUTATIONAL RESULTS FOR NONLINEAR CONSTRAINED PROBLEMS

Problem (See Reference (B6))	Number of Function and Gradient Evaluations			Number of Unconstrained Problems		
	Algorithm					
	1	2	3	1	2	3
12-1	44	33	167	3	3	5
12-3	19	24	96	2	3	4
12-5	42	62	166	3	3	5
12-8	57	49	99	3	4	5
12-10	42	31	72	2	2	4
12-14	27	74	121	2	3	5
12-15	21	30	118	2	3	4
12-17	80	120	*	5	9	*
12-18	147	193	*	7	9	*
12-23	32	45	122	3	3	5
12-25	172	174	326	7	6	9

*Did not converge to correct solution.

APPENDIX A

MATHEMATICAL CONCEPTS AND PENALTY FUNCTION TECHNIQUES

1. Introduction

Symbols, mathematical terms and related concepts are defined and briefly reviewed in this section. The topics that are directly connected with this work are alone considered. The terms and definitions are those commonly used in standard books on Nonlinear Programming (H4), (H5), (L4), (L5), (M1). A detailed information about the following concepts may be found in the above references.

2. Euclidean n-Dimensional Space

In this work real-valued functions on a set L in an Euclidean space E^n are considered. By an Euclidean space E^n is meant a linear space whose points are representable by n-tuples $\underset{\sim}{X} = (x_1, x_2, \ldots, x_n)^T$. The nonnegative orthant of E^n is denoted as E^n_+ and the positive orthant of E^n is denoted as E^n_{++}. A point is represented as a column vector *using* capital letters with underscore $\underset{\sim}{X}$, $\underset{\sim}{Y}$, ..., or lower case letters with underscore $\underset{\sim}{a}$, $\underset{\sim}{b}$, ..., or Greek letters with underscore $\underset{\sim}{\sigma}$, $\underset{\sim}{\lambda}$, ... The components of a vector are real numbers represented by lower case letters with subscript. The set of real numbers is denoted as E. The real numbers in E are represented by lower case letters a, b, ..., and Greek letters α, β, ..., without subscript or with subscript a_1, a_2, ..., α_1, α_2, ... Superscript in parentheses *is* used to represent an element of a sequence of vectors or real numbers. Subscript *is* also used to distinguish different vectors $\underset{\sim}{X}_1$, $\underset{\sim}{X}_2$, ...

A linear space E^n is a set of elements $\underset{\sim}{X}$, $\underset{\sim}{Y}$, ..., called vectors, for which the operations of addition of vectors and multiplication of vectors by scalars a, b, ... are defined and the Euclidean norm of a vector is defined as

$$\| \underset{\sim}{X} \| = (x_1{}^2 + x_2{}^2 + \dots + x_n{}^2)^{1/2} \ .$$

Linearity implies that if $a \in E$, $b \in E$, $\underset{\sim}{x} \in E^n$ and $\underset{\sim}{y} \in E^n$, then $a\underset{\sim}{x} + b\underset{\sim}{y} \in E^n$. A subspace L of E^n is a subset of E^n such that L is a linear space with the same operations as those defined in E^n and with the same scalar field. A subspace L of E^n is also called a linear manifold.

3. Sets

The set F of elements $\underset{\sim}{X}$ in E^n satisfying a property $P(\underset{\sim}{X})$ is represented as

$$F = \{\underset{\sim}{X}: \ P(\underset{\sim}{X})\}.$$

A member $\underset{\sim}{Y}$ of the set F is denoted as $\underset{\sim}{y} \in F$ and if $\underset{\sim}{Y}$ is not a member of F, then $\underset{\sim}{y} \notin F$. The union of two sets A and B in E^n is the set of elements that belong to either A or B.

$$A \subseteq B = \{\underset{\sim}{X}: \ \underset{\sim}{X} \in A \text{ or } \underset{\sim}{X} \in B\}.$$

The intersection of two sets A and B is the set of elements that belong to both A and B.

$$A \subseteq B = \{\underset{\sim}{X}: \ \underset{\sim}{X} \in A \text{ and } \underset{\sim}{X} \in B\}.$$

If every element of A is also a member of B, then A is a proper subset of B, i.e., $A \subseteq B$. If A B, then A may be a proper subset of B or may be B

itself. The complement of a set $\mathcal{A}$ is denoted as $\bar{\mathcal{A}}$ and it consists of elements not in $\mathcal{A}$. If $a \in \mathcal{E}$ and $b \in \mathcal{E}$, etc., $[a, b]$ denotes the set of real numbers $a \leqq x \leqq b$. If $x \in (a, b]$ then $a < x \leqq b$.

A real-valued function $f(\underset{\sim}{X})$ defined on a subset $\mathcal{F}$ of $\mathcal{E}^n$ is represented as $f(\underset{\sim}{X})$: $\mathcal{E}^n \rightarrow \mathcal{E}$. The minimization of $f(\underset{\sim}{X})$ over the set $\mathcal{F}$ is represented as

$$\underset{\underset{\sim}{X} \in \mathcal{F}}{\text{Minimize}} \; f(\underset{\sim}{X})$$

If $\mathcal{F}$ is the space $\mathcal{E}^n$, then the minimization is unconstrained. Otherwise the minimization is constrained.

4. Linearly Independent Set of Vectors

A set of m vectors $\underset{\sim}{X}_1, \underset{\sim}{X}_2, \ldots, \underset{\sim}{X}_m$ is said to be a set of linearly independent vectors if a relation of the form

$$a_1\underset{\sim}{X}_1 + a_2\underset{\sim}{X}_2 + \ldots + a_m\underset{\sim}{X}_m = 0$$

holds only when the scalars $a_1, a_2, \ldots, a_m$ are all zero. The vectors are linearly dependent if they are not linearly independent. A set of n linearly independent vectors is a basis for $\mathcal{E}^n$. The dimension of a space is the number of vectors in a basis for that space. Let a set of m linearly independent vectors in $\mathcal{E}^n$ define a subspace $\mathcal{B}$ of $\mathcal{E}^n$. The set of all vectors in $\mathcal{E}^n$ which are orthogonal to $\mathcal{B}$ is a subspace called the orthogonal complement of $\mathcal{B}$ and is denoted by $\mathcal{B}^1$. Any vector $\underset{\sim}{X} \in \mathcal{E}^n$ may be uniquely represented as $\underset{\sim}{X} = \underset{\sim}{Y} + \underset{\sim}{Z}$ where $\underset{\sim}{Y} \in \mathcal{B}$ and $\underset{\sim}{Z} \in \mathcal{B}^1$.

5. Characterization of Neighborhood of a Point, Sets and Sequences

5.1 Neighborhood of a Point

The ε-neighborhood of a point $\underset{\sim}{X}^*$ in $\mathcal{E}^n$ is the set of points $\underset{\sim}{X}$ lying in the open sphere or ball of radius $\varepsilon > 0$ and $\underset{\sim}{X}^*$. The ε-neighborhood of $\underset{\sim}{X}^* = \{\underset{\sim}{X}: \| \underset{\sim}{X}-\underset{\sim}{X}^* \| < \varepsilon\}$. In general it is not necessary to restrict a neighborhood of a point to be an ε-neighborhood. Therefore a neighborhood of a point $\underset{\sim}{X}^*$ is defined as any open set containing $\underset{\sim}{X}^*$.

5.2 Nature of a Point $\underset{\sim}{X}_o$ With Respect to a Set $\mathcal{F}$ in $\mathcal{E}^n$

A point $\underset{\sim}{X}_o$ is an interior point of $\mathcal{F}$ if $\mathcal{F}$ contains an ε-neighborhood of $\underset{\sim}{X}_o$. A point $\underset{\sim}{X}_o$ is an accumulation point or a limit point of $\mathcal{F}$ if every ε-neighborhood of $\underset{\sim}{X}_o$ contains a point $\underset{\sim}{X} \neq \underset{\sim}{X}_o$ belonging to $\mathcal{F}$. A limit point of $\mathcal{F}$ need not be in $\mathcal{F}$. A point $\underset{\sim}{X}_o$ is an isolated point of $\mathcal{F}$ if $\underset{\sim}{X}_o$ is in $\mathcal{F}$ but is not a limit point of $\mathcal{F}$. A point $\underset{\sim}{X}_o$ is a boundary point of $\mathcal{F}$ if every ε-neighborhood of $\underset{\sim}{X}_o$ contains points in $\mathcal{F}$ and points not in $\mathcal{F}$. A point $\underset{\sim}{X}_o$ is an exterior point of $\mathcal{F}$ if it is interior to the complement of $\mathcal{F}$.

5.3 Characterization of a Set in Terms of the Points in it

A set $\mathcal{F}$ in $\mathcal{E}^n$ is open if all of its points are interior points. Equivalently, $\mathcal{F}$ is open if given $\underset{\sim}{X} \varepsilon \mathcal{F}$ and $\exists$ and $\varepsilon > 0 \ni \| \underset{\sim}{Y}-\underset{\sim}{X} \| < \varepsilon$ implies $\underset{\sim}{Y} \varepsilon \mathcal{F}$. It is closed if it contains its limit points. Equivalently, $\mathcal{F}$ is closed if $\underset{\sim}{X}_1 \varepsilon \mathcal{F}$ and $\underset{\sim}{X}_1 \to \underset{\sim}{X}$ implies $\underset{\sim}{X} \varepsilon \mathcal{F}$. The closure of any set $\mathcal{F}$ in $\mathcal{E}^n$ is the smallest closed set containing $\mathcal{F}$. The boundary of a set is that part of the closure that is not in the interior. A set $\mathcal{F}$ is bounded if there exists a positive number r such that $\| \underset{\sim}{X} \| \leqq r$ for every $\underset{\sim}{X} \varepsilon \mathcal{F}$. A closed and bounded set is said to be compact. A neighborhood of a set $\mathcal{F}$ is an open set $\mathcal{D}$ containing $\mathcal{F}$. By an ε-neighborhood of $\mathcal{F}$ is meant a set of points each of which lies in an ε-neighborhood of some point $\underset{\sim}{X}$ in $\mathcal{F}$.

The ε-neighborhood of F is the union of the ε-neighborhoods of its points.

If $A \subseteq E$ is a bounded set of real numbers, then the smallest real number y such that $x \leq y \ \forall x \in A$ is called the least upper bound or supremum of A and is denoted as

$$y = \sup_{x \in A}(x) \text{ or } y = \sup\{x: \ x \in A\}.$$

Similarly, the greatest lower bound or infimum y of a set A is denoted as

$$y = \inf_{x \in A}(x) \text{ or } y = \inf\{x: \ x \in A\}.$$

5.4 Characterization of a Sequence

A sequence of vectors is represented as $\{\underset{\sim}{X}^{(k)}\}_{k=0}^{\infty}$ or as $\{\underset{\sim}{X}^{(k)}\}$ when the index set is implicitly understood. The sequence $\{\underset{\sim}{X}^{(k)}\}$ is said to converge to the limit $\underset{\sim}{X}^*$ if $\| \underset{\sim}{X}^{(k)} - \underset{\sim}{X}^* \| \to 0$ as $k \to \infty$. Equivalently, $\underset{\sim}{X}^*$ is the limit point of the sequence $\{\underset{\sim}{X}^{(k)}\}$ if for every $\varepsilon > 0$ there is an integer ρ such that $\underset{\sim}{X}^{(k)}$ is in the ε-neighborhood of $\underset{\sim}{X}^*$ whenever $k > \rho$. Each of the symbols

$$"\underset{\sim}{X}^{(k)} \to \underset{\sim}{X}^*", \ "\lim \underset{\sim}{X}^{(k)} = \underset{\sim}{X}^*" \text{ and } \lim_{k \to \infty} \underset{\sim}{X}^{(k)} = \underset{\sim}{X}^*$$

signifies that $\underset{\sim}{X}^*$ is the limit of the sequence $\{\underset{\sim}{X}^{(k)}\}$. If $\underset{\sim}{X}^{(k)} \to \underset{\sim}{X}^*$ and $\{\underset{\sim}{Y}^{(k)}\}$ is a subsequence of $\{\underset{\sim}{X}^{(k)}\}$, then $\underset{\sim}{Y}^{(k)} \to \underset{\sim}{X}^*$. A sequence $\{\underset{\sim}{X}^{(k)}\}$ is a Cauchy sequence if

$$\lim_{k,\ell \to \infty} \| \underset{\sim}{X}^{(k)} - \underset{\sim}{X}^{(\ell)} \| = 0.$$

A sequence $\{\underset{\sim}{X}^{(k)}\}$ in E^n converges if and only if it is a Cauchy sequence.

A sequence $\{\underset{\sim}{X}^{(k)}\}$ is bounded if there is a finite positive number r such that $\| \underset{\sim}{X}^{(k)} \| \leqq r$ for every integer k. A point $\underset{\sim}{X}^*$ is an accumulation point or a cluster point of a sequence $\{\underset{\sim}{X}^{(k)}\}$ if it is the limit of a subsequence of $\{\underset{\sim}{X}^{(k)}\}$.

A set F in E^n is closed if and only if the limits of convergent sequences in F are in F. Every bounded sequence $\{\underset{\sim}{X}^{(k)}\}$ of points in E^n possesses a convergent subsequence. Let $\{r^{(k)}\}$ be a bounded sequence of real numbers and $V^{(k)} = \sup\{r^{(i)}: \ i \geqq k\}$. Then $\{V^{(k)}\}$ converges to a real number q* called the limit superior of $\{r^{(k)}\}$ and $V^* = \lim_{k\to\infty} (r^{(k)})$.

5.4.1 Order of Convergence of a Sequence

Let $\{r^{(k)}\}$ be a sequence of real numbers converging to r*. The order of convergence of $\{r^{(k)}\}$ is defined as the supremum of nonnegative numbers p satisfying

$$0 \leqq \lim_{k\to\infty} \frac{|r^{(k+1)} - r^*|}{|r^{(k)} - r^*|p} < \infty.$$

This definition of the order of convergence is a step-wise concept as it defines bounds on the progress made in moving from kth term to (k+1)th term. The order of convergence is determined only by the properties of the sequence when k → ∞. It is a measure of the speed of convergence of the "tail" of the sequence $\{r^{(k)}\}$. A large value of p implies a high speed of convergence. If the sequence has pth order of convergence and if

$$\beta = \lim_{k\to\infty} \frac{|r^{(k+1)} - r^*|}{|r^{(k)} - r^*|p}$$

then asymptotically

$$|r^{(k+1)} - r^*| = \beta |r^{(k)} - r^*|^p.$$

When p = 2 the sequence has second order convergence.

If the sequence $\{r^{(k)}\}$ has an order of convergence equal to unity, then it is said to converge linearly to r*. The sequence converges to r* linearly with convergence ratio β if

$$\lim_{k\to\infty} \frac{|r^{(k+1)} - r^*|}{|r^{(k)} - r^*|} = \beta < 1.$$

A linearly convergent sequence with convergence ratio β is said to have a tail that converges at least as fast as the geometric sequence $\{d\beta^{(k)}\}$ for some constant d. Therefore linear convergence is sometimes referred to as geometric convergence. The smaller the convergence ratio, the faster is the rate of convergence. When p = 1 and β = 0, the rate of convergence is said to be superlinear. The convergence of any order greater than unity is also superlinear.

The average convergence rates may be used to place bounds on the average progress per step over a large number of steps. However in comparing convergence of different sequences, the step-wise convergence rates are usually used. When the sequences are well behaved and the limits involved in the definition of convergence rates exist the step-wise and average convergence rates coincide. Additional information on the convergence of sequences may be found in (L5).

The convergence properties of a sequence of vectors $\{\underset{\sim}{X}^{(k)}\}$ are defined with respect to a function that converts the sequence of vectors into a sequence of numbers. If $f(\underset{\sim}{X})$: $\mathcal{E}^n \to \mathcal{E}$ is defined on $\mathcal{E}^n$, the convergence of $\{\underset{\sim}{X}^{(k)}\}$ to $\underset{\sim}{X}^*$ can be defined in terms of the convergence of $f(\underset{\sim}{X})$ to $f(\underset{\sim}{X}^*)$. The function $f(\underset{\sim}{X})$ used in this way to measure the convergence of $\{\underset{\sim}{X}^{(k)}\}$ is called the error function.

In optimization theory, the objective function $f(\underset{\sim}{X})$ or the function $\| \underset{\sim}{X} - \underset{\sim}{X}^* \|^2$ is chosen as the error function to analyze the convergence of the sequence of intermediate solutions $\{\underset{\sim}{X}^{(k)}\}$ to $\underset{\sim}{X}^*$. The order of convergence of a sequence is insensitive to the particular error function used and hence the particular error function used to measure convergence is not really very important (L5).

The order of convergence of a sequence is a local convergence property and is a measure of the ultimate speed of convergence. It is generally used to determine the relative advantage of one algorithm to another. The global convergence property is concerned with whether starting at an arbitrary point the sequence generated will converge to a limit point or a solution.

6. Matrix Notation

A matrix with m rows and n columns is denoted as an mxn matrix. A diagonal matrix with n rows is denoted as a diagonal matrix of order n. A diagonal matrix with unity as diagonal elements is denoted as the identity matrix I. The double subscript notation is used to represent the elements of a matrix. A matrix H with elements h_{ij} is represented as $H = \{h_{ij}\}$. The transpose of a matrix B is written as B^T. A square matrix is said to be nonsingular if its determinant is not zero. The inverse of a nonsingular square matrix G is denoted as G^{-1}. A matrix N whose columns are $\underset{\sim}{X}_1$, $\underset{\sim}{X}_2$, ..., $\underset{\sim}{X}_n$

is represented as $N = [\underset{\sim}{X}_1, \underset{\sim}{X}_2, \ldots, \underset{\sim}{X}_n]$. A vector $\underset{\sim}{X} \varepsilon \mathcal{E}^n$ is a matrix with n rows and one column. A row vector is represented as the transpose of a column vector. The determinant of a matrix H is denoted as $|H|$.

7. Eigenvalues and Quadratic Forms

Let H be a square matrix of order n. A scalar λ and a nonzero vector $\underset{\sim}{X} \varepsilon \mathcal{E}^n$ satisfying $H\underset{\sim}{X} = \lambda\underset{\sim}{X}$ are said to be an eigenvalue and an eigenvector respectively of H. The number λ is the eigenvalue of H corresponding to the eigenvector $\underset{\sim}{X}$. All the eigenvalues of H are obtained by solving the characteristic polynomial of degree n in λ, $|H - I\lambda| = 0$.

If the square matrix H of order n is symmetric, i.e., $H = H^T$, then

(i) The eigenvalues of H are real.

(ii) Let λ_1 and λ_2 be distinct eigenvalues of H and $\underset{\sim}{X}_1$ and $\underset{\sim}{X}_2$ be the corresponding eigenvectors, then $\underset{\sim}{X}_1^T \underset{\sim}{X}_2 = 0$.

The matrix H is positive definite when

(a) The quadratic form $\underset{\sim}{X}^T H \underset{\sim}{X}$ is positive definite, i.e.,

$$\underset{\sim}{X}^T H \underset{\sim}{X} > 0 \ \forall \text{ nonzero } \underset{\sim}{X} \varepsilon \mathcal{E}^n.$$

(b) All its eigenvalues are positive, i.e., $\lambda_i > 0 \ \forall i$.

(c) The determinants of the leading principal minors of H are positive. The leading principal minors of H are represented as

$$H_p = \{h_{ij}\} \qquad (i,j = 1, 2, \ldots, p).$$

The matrix H is positive semidefinite when

(a) The quadratic form $\underset{\sim}{X}^T H \underset{\sim}{X}$ is positive semidefinite, i.e.,

$$\underset{\sim}{X}^T H \underset{\sim}{X} \geqq 0 \ \forall \text{ nonzero } \underset{\sim}{X} \varepsilon \mathcal{E}^n \text{ and}$$

$$\underset{\sim}{X}^T H \underset{\sim}{X} = 0 \textit{ for some nonzero } \underset{\sim}{X} \varepsilon \mathcal{E}^n.$$

(b) The eigenvalues $\lambda_i \geqq 0$ $\forall i$ and $\lambda_i = 0$ for at least one but not all i.

The leading principal minor test cannot be used to determine semidefiniteness of the matrix. H. When some of the determinants of the leading principal minors are zero, the test will not provide information about the definiteness of H.

A matrix H is indefinite when

(a) The quadratic form $\underset{\sim}{X}^T H \underset{\sim}{X}$ is indefinite, i.e., $\underset{\sim}{X}^T H \underset{\sim}{X} < 0$ for some nonzero $\underset{\sim}{X} \varepsilon E^n$ and $\underset{\sim}{X}^T H \underset{\sim}{X} > 0$ for other nonzero $\underset{\sim}{X} \varepsilon E^n$.

(b) The eigenvalues $\lambda_i < 0$ for some i and $\lambda_j > 0$ for some j.

(c) Let $|H_i|$, i = 1, 2, ..., n be determinants of the leading principal minors of H. The matrix H is indefinite if $|H_i| \neq 0$ $\forall i$ and $|H_i|/|H_{i-1}| < 0$ for some i and $|H_j|/|H_{j-1}| > 0$ for some j.

8. Norm and Condition Number of a Matrix

The norm of a square matrix H of order n, subordinate to the vector norm $\| \underset{\sim}{X} \|$, is defined as $\| H \| = \max\limits_{\| \underset{\sim}{X} \| \neq 0} \frac{\| H\underset{\sim}{X} \|}{\| \underset{\sim}{X} \|}$. The norm $\| H \|$ relative to the Euclidean norm $\| X \|$ is

$$\| H \| = \max_{\| \underset{\sim}{X} \| \neq 0} \left[\frac{\underset{\sim}{X}^T H^T H\underset{\sim}{X}}{\underset{\sim}{X}^T \underset{\sim}{X}}\right]^{1/2}, \quad \underset{\sim}{X} \varepsilon E^n.$$

Therefore the norm $\| H \|$ relative to the Euclidean norm of a vector $\underset{\sim}{X}$ in E^n is the square root of the largest eigenvalue of $H^T H$. If H is a symmetric matrix, then $\| H \|$ is the largest eigenvalue of H and $\| H^{-1} \|$ is the reciprocal of the smallest eigenvalue of H. Let λ_ℓ and λ_s be the largest and smallest eigenvalues of H. Then the condition number r of the matrix

H is defined as $r = \lambda_\ell/\lambda_s$. The matrix H is said to be well-conditioned if the value of r is close to 1. If the value of r is very large, the matrix H is said to be ill-conditioned. The ill-conditioning of H increases as the value of r increases.

9. Functions

A real valued function $f(\underset{\sim}{X})$ defined on a subset L of E^n is represented as $f(\underset{\sim}{X})$: $E^n \rightarrow E$. A function $f(\underset{\sim}{X})$ is said to be continuous on a set L if it is continuous at each point $\underset{\sim}{X_o}$ in L. It is continuous at a point $\underset{\sim}{X_o}$ in L if $f(\underset{\sim}{X}) \rightarrow f(\underset{\sim}{X_o})$ whenever $\underset{\sim}{X} \varepsilon L$ and $\underset{\sim}{X} \rightarrow \underset{\sim}{X_o}$. Equivalently, $f(\underset{\sim}{X})$ is continuous at $\underset{\sim}{X_o}$ if given $\varepsilon > 0$ there is a $\delta > 0$ such that $\| \underset{\sim}{X} - \underset{\sim}{X_o} \| < \delta$ implies $|f(\underset{\sim}{X}) - f(\underset{\sim}{X_o})| < \varepsilon$. A set of real-valued functions $c_i(\underset{\sim}{X})$, $i = 1, 2, \ldots, m$ may be regarded as a single vector function $\underset{\sim}{C}(\underset{\sim}{X})$: $E^n \rightarrow E^m$. Such a vector function is said to be continuous on an open set $L \subseteq E^n$ if each of its component functions is continuous on L.

A real valued function $f(\underset{\sim}{X})$ is said to be of class $C^{(k)}$ or $f \varepsilon C^{(k)}$ on an open set $L \subseteq E^n$ if it is continuous and possesses continuous partial derivatives of all orders $\leqq$ k. If $f \varepsilon C^{(k+1)}$ on L, it is of class $C^{(k)}$ on L. The gradient of $f \varepsilon C^{(1)}$ at $\underset{\sim}{X}^*$ is the column vector

$$\underset{\sim}{\nabla} f(\underset{\sim}{X}^*) = [\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n}]^T_{\underset{\sim}{X}^*}.$$

If $f \varepsilon C^{(2)}$, the Hessian of f at $\underset{\sim}{X}^*$ is the square symmetric matrix of order n denoted as $\nabla^2 f(\underset{\sim}{X}^*)$ or $F(\underset{\sim}{X}^*)$

$$\nabla^2 f(\underset{\sim}{X}^*) = \{\frac{\partial f}{\partial x_i \, \partial x_j}\}_{\underset{\sim}{X}^*} = \{f_{ij}\}_{\underset{\sim}{X}^*} \quad i,j = 1, 2, \ldots, n.$$

If the vector-valued function $\underset{\sim}{C}(\underset{\sim}{X})$: $\mathcal{E}^n \rightarrow \mathcal{E}^m$ is of class $C^{(1)}$, its gradient at $\underset{\sim}{X}^*$ is the mxn matrix, $\nabla \underset{\sim}{C}(\underset{\sim}{X}) = \{\frac{\partial C_i}{\partial x_j}\}_{\underset{\sim}{X}^*}$ $\forall i, j = 1, 2, \ldots, n$, called Jacobian of $\underset{\sim}{C}$ at $\underset{\sim}{X}^*$. If a vector $\underset{\sim}{\lambda}\ \varepsilon\ \mathcal{E}^m$ and if the real-valued function $\underset{\sim}{\lambda}^T C$: $\mathcal{E}^{m+n} \rightarrow \mathcal{E}$ is of class $C^{(2)}$, the gradient of $\underset{\sim}{\lambda}^T \underset{\sim}{C}$ at any point $\underset{\sim}{X}$ is

$$\underset{\sim}{\nabla}[\underset{\sim}{\lambda}^T \underset{\sim}{C}] = [\nabla \underset{\sim}{C}]^T\ \underset{\sim}{\lambda}.$$

The Hessian of $\underset{\sim}{\lambda}^T \underset{\sim}{C}$ at any point $\underset{\sim}{X}$ is equal to $\sum_{i=1}^{m} \lambda_i\ \nabla^2 C_i(\underset{\sim}{X})$.

The set of points satisfying the equation $f(\underset{\sim}{X}) = c$, where $c\ \varepsilon\ \mathcal{E}$ and f: $\mathcal{E}^n \rightarrow \mathcal{E}$, forms a level surface of f. If f is of the form $f(\underset{\sim}{X}) = \sum_{i=1}^{n} a_i\ x_i + b$, a_i not all zero, then the level surfaces of f are (n-1) dimensional hyperplanes and $\underset{\sim}{\nabla} f$ is the normal to the hyperplanes. In general, if $f\ \varepsilon\ C^{(1)}$ and $\underset{\sim}{\nabla} f \neq 0$ at $\underset{\sim}{X}_o$ in $\mathcal{L}$, then $\underset{\sim}{\nabla} f(\underset{\sim}{X}_o)$ is the normal at $\underset{\sim}{X}_o$ to the level surface $f(\underset{\sim}{X}) = f(\underset{\sim}{X}_o)$. If $f\ \varepsilon\ C^{(2)}$, $\underset{\sim}{d}$ is a direction vector in $\mathcal{E}^n$ and F is the Hessian of f, then the directional derivative of f at a point $\underset{\sim}{X}$ in the direction $\underset{\sim}{d}$ is $\underset{\sim}{d}^T \underset{\sim}{\nabla} f$ and the second derivative of f in that direction is $\underset{\sim}{d}^T\ F\ \underset{\sim}{d}$.

Let $f\ \varepsilon\ C^{(2)}$ be defined on an open set $\mathcal{L} \subseteq \mathcal{E}^n$ and $\underset{\sim}{X}_1\ \varepsilon\ \mathcal{L}$. In an open neighborhood of $\underset{\sim}{X}_1$, f may be represented using the following Taylor series

$$f(\underset{\sim}{X}) = f(\underset{\sim}{X}_1) + (\underset{\sim}{X}-\underset{\sim}{X}_1)^T\ \nabla f(\underset{\sim}{X}_1) + \frac{1}{2}\ (\underset{\sim}{X}-\underset{\sim}{X}_1)^T\ \nabla^2 f(\underset{\sim}{X}_1)(\underset{\sim}{X}-\underset{\sim}{X}_1)$$

$$+\ r(\underset{\sim}{X}_1,\ \underset{\sim}{X}-\underset{\sim}{X}_1)$$

where $r(\underset{\sim}{X}_1,\ \underset{\sim}{X}-\underset{\sim}{X}_1)$ is the remainder term. The remainder term satisfies the relation (H4)

$$\lim_{\Delta \underset{\sim}{X} \rightarrow 0} \frac{r(\underset{\sim}{X}_1,\ \Delta \underset{\sim}{X})}{\|\ \Delta \underset{\sim}{X}\ \|^2} = 0 \text{ where } \Delta \underset{\sim}{X} = \underset{\sim}{X} - \underset{\sim}{X}_1.$$

Therefore the quadratic approximation to $f(\underset{\sim}{X})$ about $\underset{\sim}{X}_1$ is the Taylor series

$$f(\underset{\sim}{X}) = f(\underset{\sim}{X}_1) + \Delta\underset{\sim}{X}^T \, \nabla f(\underset{\sim}{X}_1) + \frac{1}{2} \, \Delta\underset{\sim}{X}^T \, \nabla^2 f(\underset{\sim}{X}_1) \, \Delta\underset{\sim}{X}, \; \Delta\underset{\sim}{X} = \underset{\sim}{X} - \underset{\sim}{X}_1.$$

10. Implicit Function Theorem

The implicit function theorem is concerned with the conditions under which a set of equations $g_i(\underset{\sim}{X}, \underset{\sim}{\lambda}) = 0 \quad i = 1, 2, \ldots, n, \; \underset{\sim}{X} \varepsilon \, E^n, \; \underset{\sim}{\lambda} \varepsilon \, E^m$, $g_i\colon \; E^{n+M} \to E \; \forall i$ can be solved for $\underset{\sim}{X}$ as a function of $\underset{\sim}{\lambda}$, i.e., as $\underset{\sim}{X}(\underset{\sim}{\lambda})$. Let $g_i \; \forall i$ be continuous and have continuous first and second order partial derivatives with respect to $\underset{\sim}{X}$ on an open set $B \quad E^{n+m}$. Let $\underset{\sim}{g}\colon \; E^{n+m} \to E^n$ be a vector-valued function with g_i as elements. Let $\underset{\sim\sim}{\nabla g}$ be the nxn Jacobian matrix of $\underset{\sim}{g}$ with respect to $\underset{\sim}{X}$.

Suppose that $g_i(\underset{\sim}{X}, \underset{\sim}{\lambda}) = 0 \quad i = 1, 2, \ldots, n$ and $|\underset{\sim\sim}{\nabla g}| \neq 0$ at a point $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ in B. Then there exists a continuous function $\underset{\sim}{X}(\underset{\sim}{\lambda})$ on a neighborhood $A \subseteq E^m$ of $\underset{\sim}{\lambda}^*$ and a constant $\varepsilon > 0$ such that $\underset{\sim}{X}(\underset{\sim}{\lambda}^*) = \underset{\sim}{X}^*$, $g_i(\underset{\sim}{X}(\underset{\sim}{\lambda}), \underset{\sim}{\lambda}) = 0 \; \forall i$, $\underset{\sim}{\lambda} \varepsilon \, A$. Further $g_i(\underset{\sim}{X}, \underset{\sim}{\lambda}) = 0$, $\| \underset{\sim}{X} - \underset{\sim}{X}(\underset{\sim}{\lambda}) \| < \varepsilon$, $\underset{\sim}{\lambda} \varepsilon \, A$ only when $\underset{\sim}{X} = \underset{\sim}{X}(\underset{\sim}{\lambda})$. If the functions $g_i(\underset{\sim}{X}, \underset{\sim}{\lambda}) \; \forall i$ are of class $C^{(2)}$ on B, then the function $\underset{\sim}{X}(\underset{\sim}{\lambda})$ is also of class $C^{(2)}$ on A.

11. Local and Global Minima of a Function on a Set

Let $f(\underset{\sim}{X})\colon \; E^n \to E$ be defined on an open bounded set $L \subseteq E^n$. A point $\underset{\sim}{X}^* \varepsilon \, L$ is said to be a relative minimum point or a local minimum point of f over L if there is an $\varepsilon > 0$ such that $f(\underset{\sim}{X}^*) \leq f(\underset{\sim}{X}) \; \forall \; \underset{\sim}{X} \varepsilon \, L$ and $\| \underset{\sim}{X} - \underset{\sim}{X}^* \| < \varepsilon$. The point $\underset{\sim}{X}^*$ is said to be a strict local minimum point or strict relative minimum point or an isolated local minimum point of f over if there exists an $\varepsilon > 0$ such that

$$f(\underset{\sim}{X}^*) < f(\underset{\sim}{X}) \; \forall \; \underset{\sim}{X} \varepsilon \, L, \; \underset{\sim}{X} \neq \underset{\sim}{X}^* \text{ and } \| \underset{\sim}{X} - \underset{\sim}{X}^* \| < \varepsilon.$$

A point $\underset{\sim}{X}^* \varepsilon L$ is said to be a global minimum point of f over L if $f(\underset{\sim}{X}^*) \leqq f(\underset{\sim}{X})\ \forall\ \underset{\sim}{X}\ \varepsilon\ L$. The point $\underset{\sim}{X}^*$ is said to be a strict global minimum point of f over L if

$$f(\underset{\sim}{X}^*) < f(\underset{\sim}{X})\ \forall\ \underset{\sim}{X}\ \varepsilon\ L,\ \underset{\sim}{X} \neq \underset{\sim}{X}^*.$$

A point $\underset{\sim}{X}^*$ is a local (global) maximum point of $f(\underset{\sim}{X})$ over L if it is a local (global) minimum point of $-f(\underset{\sim}{X})$. A point that maximizes or minimizes f on L is called an extreme point of f on L.

12. Infimum and Supremum of a Function on a Set

Let $f(\underset{\sim}{X})\colon\ E^n \to E$ be defined on an open bounded set $L \subseteq E^n$. The infimum of f on L is the greatest lower bound of f on S. It is the largest number, $-\infty \leqq \alpha \leqq \infty$, such that $f(\underset{\sim}{X}) \geqq \alpha$ holds for all $\underset{\sim}{X}\ \varepsilon\ L$. It is denoted as "$\inf\limits_{\underset{\sim}{X}\varepsilon L} f(\underset{\sim}{X})$" or "inf $f(\underset{\sim}{X})$ on L" or "inf $f(\underset{\sim}{X})$". Equivalently,

$$\alpha = \inf \{f(\underset{\sim}{X})\colon\ \underset{\sim}{X}\ \varepsilon\ L\} \text{ if}$$

(i) $\alpha \leqq f(\underset{\sim}{X})\ \forall\ \underset{\sim}{X}\ \varepsilon\ L$

(ii) there is a sequence $\{\underset{\sim}{X}^{(k)}\}\ \varepsilon\ L$ such that

$$\lim_{k\to\infty} f(\underset{\sim}{X}^{(k)}) = \alpha$$

A point $\underset{\sim}{X}^*$ in L minimizes $f(\underset{\sim}{X})$ on L if and only if $f(\underset{\sim}{X}^*) = \inf f(\underset{\sim}{X})$. When a minimizing point $\underset{\sim}{X}^*\ \varepsilon\ L$ exists, $f(\underset{\sim}{X}^*)$ is the infimum as well as the minimum of $f(\underset{\sim}{X})$ on L. If $f(\underset{\sim}{X})\colon\ E^n \to E$ is a continuous function defined on a compact set $F \subseteq E^n$, then there exists a point $\underset{\sim}{X}^*$ such that $f(\underset{\sim}{X}^*) =$ inf $f(\underset{\sim}{X})$ on L.

The supremum of f over $\mathcal{L}$ is the least upper bound of f on $\mathcal{L}$. It is the smallest real number, $-\infty \leqq \beta \leqq \infty$, such that $f(\underset{\sim}{X}) \leqq \beta \ \forall \ \underset{\sim}{X} \in \mathcal{L}$. It is denoted as "$\sup\limits_{\underset{\sim}{X} \in \mathcal{L}} f(X)$" or "$\sup f(\underset{\sim}{X})$" or "sup f(X) on $\mathcal{L}$". Equivalently,

$$\sup\{f(\underset{\sim}{X}): \ \underset{\sim}{X} \in \mathcal{L}\} = \inf\{-f(\underset{\sim}{X}): \ \underset{\sim}{X} \in \mathcal{L}\}.$$

A point $\underset{\sim}{X}^*$ maximizes $f(\underset{\sim}{X})$ on $\mathcal{L}$ if and only if $f(\underset{\sim}{X}^*) = \sup f(\underset{\sim}{X})$.

13. Convex Sets and Convex Functions

13.1 Convex Sets

A set $\mathcal{F} \subseteq \mathcal{E}^n$ is said to be a convex set if for every $\underset{\sim}{X}_1, \underset{\sim}{X}_2 \in \mathcal{F}$ and $0 < \alpha < 1$,

$$\alpha \underset{\sim}{X}_1 + (1-\alpha) \underset{\sim}{X}_2 \in \mathcal{F}.$$

Geometrically, a set is a convex set if the line segment joining any two points in the set lies in the interior of that set. If $\beta \underset{\sim}{X}_1 + (1-\beta) \underset{\sim}{X}_2 \in \mathcal{F}$ for every $\underset{\sim}{X}_1, \underset{\sim}{X}_2 \in \mathcal{F}$ and $\beta \in \mathcal{E}$, then the set $\mathcal{F}$ is said to be an affine set or a linear variety.

The closure of a convex set is convex. The intersection and union of any number of convex sets is convex. The null set is assumed to be convex. The convex set defined by every convex linear combination of a finite number of points in $\mathcal{E}^n$ is a simplex in $\mathcal{E}^n$. The convex hull of a set S is the smallest convex set containing S. The closure of a convex hull of S is the closed convex hull of S.

13.2 Convex and Concave Functions

A function $f(\underset{\sim}{X})$: $E^n \to E$ defined on a convex set L is said to be convex on L if for every $\underset{\sim}{X}_1, \underset{\sim}{X}_2 \in L$ and $0 \leqq \alpha \leqq 1$,

$$f(\alpha \underset{\sim}{X}_1 + (1-\alpha)\ \underset{\sim}{X}_2) \leqq \alpha f(\underset{\sim}{X}_1) + (1-\alpha)\ f(\underset{\sim}{X}_2).$$

If for $\underset{\sim}{X}_1 \neq \underset{\sim}{X}_2$, $0 < \alpha < 1$, $\underset{\sim}{X}_1, \underset{\sim}{X}_2 \in L$

$$f(\alpha \underset{\sim}{X}_1 + (1-\alpha)\ \underset{\sim}{X}_2) < \alpha f(\underset{\sim}{X}_1) + (1-\alpha)\ f(\underset{\sim}{X}_2),$$

then $f(\underset{\sim}{X})$ is said to be strictly convex on L. A function $f(\underset{\sim}{X})$ is said to be (strictly) concave on L if $-f(\underset{\sim}{X})$ is (strictly) convex on L. A positive linear combination of convex functions is convex.

If $f(\underset{\sim}{X})$: $E^n \to E$ defined on a convex set $L \subseteq E^n$ is of class $C^{(1)}$ on L, then $f(\underset{\sim}{X})$ is convex on L if and only if

$$f(\underset{\sim}{X}_2) \geqq f(\underset{\sim}{X}_1) + \underset{\sim}{\nabla} f(\underset{\sim}{X}_1)\ (\underset{\sim}{X}_2 - \underset{\sim}{X}_1)$$

for all points $\underset{\sim}{X}_1, \underset{\sim}{X}_2 \in L$.

If for all $\underset{\sim}{X}_1, \underset{\sim}{X}_2 \in L$,

$$f(\underset{\sim}{X}_2) > f(\underset{\sim}{X}_1) + \underset{\sim}{\nabla} f(\underset{\sim}{X}_1)\ (\underset{\sim}{X}_1 - \underset{\sim}{X}_2)$$

then f is strictly convex on L. If $f(\underset{\sim}{X})$ is of class $C^{(2)}$ on a convex set L, then $f(\underset{\sim}{X})$ is convex on L if and only if at each point $\underset{\sim}{X} \in L$ the Hessian matrix F of f is positive semidefinite. If F is positive definite $\forall\ \underset{\sim}{X} \in L$, then f is strictly convex on L.

13.3 Convex Sets Defined by Convex and Concave Functions

Let $f(\underset{\sim}{X})$: $\mathcal{E}^n \rightarrow \mathcal{E}$ be a convex function defined on a convex set $\mathcal{L}$. The set $\mathcal{F} = \{\underset{\sim}{X}\text{:}\ \ f(\underset{\sim}{X}) \leqq \alpha,\ \underset{\sim}{X} \in \mathcal{L}\}$ is a convex set for every $\alpha \in \mathcal{E}$. If $f(\underset{\sim}{X})$ is a concave function defined on a convex set $\mathcal{L}$, then the set

$$\mathcal{F} = \{\underset{\sim}{X}\text{:}\ \ f(\underset{\sim}{X}) \geqq \alpha,\ \underset{\sim}{X} \in \mathcal{L}\}$$

is a convex set for every $\alpha \in \mathcal{E}$.

If $f(\underset{\sim}{X})$ is linear or affine, then $f(\underset{\sim}{X}) < \alpha$ defines an open half space, $f(\underset{\sim}{X}) \leqq \alpha$ defines a closed half space and $f(\underset{\sim}{X}) = 0$ defines an $(n-1)$ dimensional hyperplane. The intersection of a finite number of closed half spaces is a convex polytope. A nonempty bounded convex polytope is a convex polyhedron. A convex set may be defined by linear equalities. However nonlinear equalities cannot define a convex set. A detailed treatment of convex sets and convex functions may be found in references (H4), (L5), (M1), (R1), (Z1), (Z2).

14. Penalty and Barrier Function Methods

Consider the inequality constrained problem P1. The feasible region $\mathcal{F}$ is defined as follows.

$$\mathcal{F} = \{\underset{\sim}{X}\text{:}\ \ c_i(\underset{\sim}{X}) \geqq 0,\ 1 \leqq i \leqq m\}.$$

The interior of the feasible region $\mathcal{F}$ is defined as

$$\mathcal{F}_I = \{\underset{\sim}{X}\text{:}\ \ c_i(\underset{\sim}{X}) > 0,\ 1 \leqq i \leqq m\}.$$

The exterior of the feasible region $\mathcal{F}$ is denoted as $\overline{\mathcal{F}}$.

14.1 Barrier Function Method

The barrier function method is a transformation technique. The barrier function transformation for P1 may be represented as

$$B(\underset{\sim}{X},\mu) = f(\underset{\sim}{X}) + \sum_{i=}^{m} P_i(C_i(\underset{\sim}{X})), \ \mu > 0.$$

The function $B(\underset{\sim}{X},\mu)$ is defined so that a barrier is constructed at the boundary of the feasible region F. A solution $\underset{\sim}{X}^*$ to P1 is approached from the set F_I by modifying the barrier function using the control parameter μ. The set F_I is assumed to be nonempty and this means that any boundary point of F may be approached from a point in the set F. This also implies that the barrier function is not a suitable transformation for equality constraints.

In the function $B(\underset{\sim}{X},\mu)$, the second term is the barrier term. For $\mu > 0$, this term is bounded and is defined continuously on the interval $c_i(\underset{\sim}{X}) > 0$. Further $\rho_i(t) \to \infty$, as $t \to 0_+$. The commonly used barrier functions are (F1), (R11)

(i) The inverse barrier function $\rho_i(c_i(\underset{\sim}{X})) = (c_i(\underset{\sim}{X}))^{-1}$.

(ii) The logarithmic barrier function $\rho_i(c_i(\underset{\sim}{X}) = -\ell n(c_i(\underset{\sim}{X}))$.

The function $B(\underset{\sim}{X},\mu)$ is defined on F_I and twice continuously differentiable in F_I. Further $B(\underset{\sim}{X},\mu) \geqq 0$ and $B(\underset{\sim}{X},\mu) \to \infty$ as $c_i(X^*) \to 0$ for any i. Therefore a barrier is established at the boundary of the feasible region. This barrier prevents a search procedure for locating a solution $\underset{\sim}{X}^*$ to P1 from leaving the feasible region. As $B(\underset{\sim}{X},\mu)$ is defined on F_I and the method operates in F_I, the barrier function method is also called an interior-point method. If $c_i(\underset{\sim}{X}^*) = 0$, then as $\underset{\sim}{X} \to X^*$, the growth of $\rho_i(c_i(\underset{\sim}{X}))$ is controlled or cancelled by decreasing μ.

The barrier function method may be summarized as follows. Select a sequence $\{\mu^{(k)}\}$ such that for each k,

$$\mu^{(k)} > 0, \mu^{(k+1)} < \mu^{(k)} \text{ and } \lim_{k\to\infty} \mu^{(k)} = 0.$$

For each k, minimize $B(\underset{\sim}{X}, \mu^{(k)})$ to find $\underset{\sim}{X}^{(k)} = \underset{\sim}{X}(\mu^{(k)})$, starting the unconstrained minimization from $\underset{\sim}{X}^{(k-1)}$. The initial starting point $\underset{\sim}{X}^{(0)}$ must be in $\mathcal{F}_I$. The stopping criteria for each unconstrained minimization may be based on $|f(\underset{\sim}{X}^{(k)}) - f(\underset{\sim}{X}^{(k-1)})|$ or $\| \underset{\sim}{X}^{(k)} - \underset{\sim}{X}^{(k-1)} \|$.

Let $\{\underset{\sim}{X}^{(k)}\}$ be the sequence generated by the method. Then any limit point of this sequence is optimal for P1 (Z1). The behavior of $B(\underset{\sim}{X},\mu)$ may be interpreted in the following way (R11). Let $c_i(\underset{\sim}{X}^*) = 0$ for some i. As $\underset{\sim}{X}^{(k)} \to \underset{\sim}{X}^*$, $c_i(\underset{\sim}{X}^{(k)}) \to c_i(X^*) = 0$, $\rho_i(c_i(\underset{\sim}{X}^{(k)})) \to \infty$ and $B(\underset{\sim}{X}^{(k)},\mu) \to \infty$. However if μ is decreased, then $\rho_i(c_i(\underset{\sim}{X}^{(k)}))$ can be allowed to increase without increasing $B(\underset{\sim}{X}^{(k)},\mu)$. The monotonically decreasing sequence $\{\mu^{(k)}\}$ is chosen in such a way that

(i) $B(\underset{\sim}{X}^{(k)}, \mu^{(k)})$ monotonically decreases.

(ii) $B(\underset{\sim}{X}, \mu^{(k)})$ is twice continuously differentiable in $\mathcal{F}_I$.

(iii) $c_i(\underset{\sim}{X}^{(k)}) \to 0$, $\underset{\sim}{X}^{(k)} \to \underset{\sim}{X}^*$, and $f(\underset{\sim}{X}^{(k)}) \to f(\underset{\sim}{X}^*)$.

As the search for $\underset{\sim}{X}^*$ is started at $\underset{\sim}{X}^{(0)} \in \mathcal{F}_I$, the barrier at the boundary of $\mathcal{F}$ restricts the search procedure and the sequence, $\{\underset{\sim}{X}^{(k)}\}$, of minimizing points of $B(\underset{\sim}{X}, \mu^{(k)})$ to the interior of $\mathcal{F}$. The method is therefore called an interior-point method.

The strengths and weaknesses of the method are discussed in detail in reference (R11). The method facilitates the solution of P1 using an unconstrained minimization technique and the constraints need not be accounted for explicitly. The convergence of the method has been established (F1) when the problem functions are continuous and $\underset{\sim}{X}^*$ is at the boundary of $\mathcal{F}$ or in the closure of $\mathcal{F}_I$. Fiacco and McCormick (F1) established that there exist a sequence $\{\mu^{(k)}\}$ and a corresponding sequence of minimizing points generated by the algorithm such that $\underset{\sim}{X}^{(k)} \rightarrow \underset{\sim}{X}^*$ as $k \rightarrow \infty$. Similar convergence properties and convergence of the other related sequences have been proved by Luenberger (L5) and Zangwill (Z1).

The method does not require very strong constraint qualifications and *it converges to a local minimum of P1 where the Kuhn-Tucker conditions may* or may not hold. By *monitoring the convergence of the sequences* $\{\underset{\sim}{C}(\underset{\sim}{X}^{(k)})\}$ and $\{\underset{\sim}{\lambda}^{(k)}\}$, structural information about the problem P1 may be obtained. The most commonly sought structural information is the set of active constraints at $\underset{\sim}{X}^{(k)}$. The vector $\underset{\sim}{\lambda}^{(k)}$ is an estimate of $\underset{\sim}{X}^{(k)}$ of the Lagrange multiplier vector $\underset{\sim}{\lambda}^*$ at $\underset{\sim}{X}^*$. The method converges even when the minimization of $B(\underset{\sim}{X}, \mu^{(k)})$ is inexact for each k (R11).

The weaknesses of the barrier function method are of a computational nature and are most serious when the controlling parameter μ is small. The numerical difficulties associated with the algorithm arise due to the ill-conditioning of the Hessian of $B(\underset{\sim}{X}, \mu^{(k)})$. The condition number of the Hessian of $B(\underset{\sim}{X}, \mu^{(k)})$ increases as decreases. This causes $B(\underset{\sim}{X}, \mu^{(k)})$ to have steep-sided valleys and makes the search for an unconstrained minimum of $B(\underset{\sim}{X}, \mu^{(k)})$ difficult. In the algorithm, $\mu^{(k)}$ is gradually decreased so as to make $B(\underset{\sim}{X}, \mu^{(k)})$ twice continuously differentiable and to reduce the ill-conditioning of the Hessian of $B(\underset{\sim}{X}, \mu^{(k)})$. The feature that restricts the general application of the method is that it requires the initial point to be feasible and the search for $\underset{\sim}{X}^{(0)}$ is as difficult as the problem to be solved. Further the method cannot handle equality constraints.

14.2 Penalty Function Method

The penalty function transformation for P1 may be represented as

$$P(\underset{\sim}{X}, \sigma) = f(\underset{\sim}{X}) + \sigma \sum_{i=1}^{m} \eta_i(c_i(\underset{\sim}{X})), \quad \sigma > 0.$$

The properties of the loss functions $\eta_i(c_i(\underset{\sim}{X}))$ and $P(\underset{\sim}{X}, \sigma)$ are discussed in detail in Chapter 2. Additional information may be found in references (F1), (L5), (Z1), (Z2). The penalty function designed to impose an increasing penalty on the objective function as the search point $\underset{\sim}{X}$ moves away from F and the constraint violation increases. The loss functions $\eta_i(t)$ are defined for $-\infty < t < \infty$ and therefore the penalty function is defined on E^n. This implies that both equality and inequality constraints can be handled by the penalty function transformation technique. When $\underset{\sim}{X} \in F$, the loss term is zero and when $\underset{\sim}{X} \notin F$ penalty is imposed on $F(\underset{\sim}{X})$ depending on how far $\underset{\sim}{X}$ is away from F. Therefore the algorithm may be started at any $\underset{\sim}{X}^{(0)} \in E^n$ and specially $\underset{\sim}{X}^{(0)} \in F$ or $\underset{\sim}{X}^{(0)} \in F$.

The loss functions η_i $\forall i$ are usually chosen so that $P(\underset{\sim}{X}, \sigma)$ is twice differentiable. However the following loss functions also are used in some algorithms.

(i) Zangwill's loss function for inequalities $c_i(\underset{\sim}{X}) \geqq 0$

$$\eta_i(c_i(\underset{\sim}{X})) = -\min\ (0, c_i(\underset{\sim}{X}))$$

(ii) Absolute value loss function for equalities $c_i(\underset{\sim}{X}) = 0$

$$\eta_i(c_i(\underset{\sim}{X})) = |c_i(\underset{\sim}{X})|$$

The basic penalty function algorithm is described in Chapter 2.

The use of monotonically increasing control parameter $\sigma^{(k)}$ in the algorithm may be interpreted as follows. When $\underset{\sim}{X}^{(k)}$ is in $\mathcal{F}$, the increase in $\sigma^{(k)}$ increases the penalty weight associated with the loss term $\sigma^{(k)} \sum_i \eta_i(c_i(\underset{\sim}{X}))$. Due to this increase in the penalty weight associated with the loss term, in the subsequent unconstrained minimization of $P(\underset{\sim}{X}, \sigma^{(k+1)})$ the loss term is reduced and hence $c_i(\underset{\sim}{X}^{(k)}) \rightarrow 0$, permitting $\underset{\sim}{X}^{(k)} \rightarrow \underset{\sim}{X}^*$. The structure of $P(\underset{\sim}{X}, \sigma)$ also implies that for large σ, the minimum of $P(\underset{\sim}{X}, \sigma)$ will be in a region where $\sigma \sum_i \eta_i(c_i(\underset{\sim}{X}))$ is small. The gradual increase in σ is designed to make $P(\underset{\sim}{X}, \sigma)$ continuously differentiable and reduce the ill-conditioning of the Hessian of $P(\underset{\sim}{X}, \sigma)$.

The convergence of $\underset{\sim}{X}^{(k)}$ to $\underset{\sim}{X}^*$ and the existence of a corresponding monotonically increasing sequence $\{\sigma^{(k)}\}$ have been established by Fiacco and McCormick (F1), Luenberger (L5), Zangwill (Z1). The condition number of the Hessian of P increases as σ increases. The penalty function $P(\underset{\sim}{X}, \sigma)$ forms increasingly steep-sided valley as σ increases and this leads to numerical instabilities in the unconstrained minimization of $P(\underset{\sim}{X}, \sigma)$. Due to this reason, it is not possible to solve P1 in one step via $P(\underset{\sim}{X}, \sigma)$ by choosing a large σ. The gradual increase in σ makes the successive unconstrained minimization problems easily to solve. In the penalty function method the solution $\underset{\sim}{X}^*$ is approached from outside $\mathcal{F}$ and therefore the method also is known as the exterior-point method. Lootsma (L3) has comprehensively reviewed and classified the loss functions and barrier functions. Duality analysis of the methods is developed in references (F1), (L5) and (Z1).

14.3 Mixed Interior Point - Exterior Point Method

Fiacco and McCormick (F1) proposed and developed a mixed interior point - exterior point method for solving P3. The equality constraints are handled by the penalty function method and inequalities are taken into account using the barrier function method. The methods that solve a constrained problem by sequential unconstrained minimizations were termed Sequential Unconstrained Minimization Techniques (SUMT) by Fiacco and McCormick (F1). The most popular form of SUMT uses a quadratic loss function to handle equalities and a logarithmic barrier function for inequalities.

$$P(\underset{\sim}{X}, \sigma) = f(\underset{\sim}{X}) = \frac{1}{\sigma} \sum_{i \notin \mathcal{E}} \ln c_i(\underset{\sim}{X}) + \sigma \sum_{i \in \mathcal{E}} (c_i(\underset{\sim}{X}))^2 \quad \sigma > 0.$$

In the above function $\mathcal{E}$ is the index set of equality constraints. The properties of the mixed function are the same those reviewed above for penalty and barrier transformations. The sequence $\underset{\sim}{X}^{(k)}$ converges to $\underset{\sim}{X}^*$ when $\sigma \to \infty$. Additional information about the properties, convergence and computational considerations of the mixed methods may be found in reference (L3), (F1).

15. Duality Theory and Duality Gap

15.1 The Primal Problem

Let the primal problem be defined as follows.

$$P: \text{ Minimize } f(\underset{\sim}{X}), \ \underset{\sim}{X} \in \mathcal{L} \leq \mathcal{E}^n$$

subject to $c_i(\underset{\sim}{X}) \geqq 0 \quad i = 1, 2, \ldots, m$

$$f(\underset{\sim}{X}): \ \mathcal{E}^n \to \mathcal{E}, \quad c_i(\underset{\sim}{X}): \ \mathcal{E}^n \to \mathcal{E} \ \ \forall i.$$

The problem functions are defined on the nonempty open convex set L. The problem P is assumed to have at least one feasible solution and the set

$$\{\underset{\sim}{X}:\ \underset{\sim}{X} \in L,\ \ c_i(\underset{\sim}{X}) > \alpha_i\}$$

in E^n is compact and nonnull for every choice of $\alpha_i \in E_+$. These assumptions imply that a finite optimal value of P is attained in the feasible region F (R13). Equivalently, $-\infty < \min\ (P) < \infty$. The optimal value of P, in general, is inf (P). Equivalently, the optimal value of P is the inf $f(\underset{\sim}{X})$ subject to $\underset{\sim}{X} \in L$ and $c_i(\underset{\sim}{X}) \geqq 0$. However, if $\underset{\sim}{X}^*$ is a minimizer of P in F, then min (P) = inf (P). The conditions imposed on P imply the existence of a solution $\underset{\sim}{X}^*$ to P. Therefore in subsequent discussions the optimal value of P is denoted as min (P).

The classical Lagrangian, $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$, associated with P is defined as follows (R13).

$$L(\underset{\sim}{X}, \underset{\sim}{\lambda}):\ \ E^{n+m} \rightarrow E$$

$$L(\underset{\sim}{X}, \underset{\sim}{\lambda}) = \begin{cases} f(\underset{\sim}{X}) - \underset{\sim}{\lambda}^T\ \underset{\sim}{C}(\underset{\sim}{X}), & \underset{\sim}{\lambda} \in E_+^m \\ -\infty \text{ otherwise} & \end{cases}$$

Since $f(\underset{\sim}{X}) \geqq L(\underset{\sim}{X}, \underset{\sim}{\lambda})$, $\sup L(\underset{\sim}{X}, \underset{\sim}{\lambda}) = f(\underset{\sim}{X})$ when $\underset{\sim}{X}$ is feasible. The optimal value of P also may be represented as

$$\min\ (P) = \inf\ (P) = \inf_{\underset{\sim}{X} \in L}\ \sup_{\underset{\sim}{\lambda} \in E^m}\ L(\underset{\sim}{X}, \underset{\sim}{\lambda}).$$

A vector $\underset{\sim}{\lambda}^*$ is a Kuhn-Tucker vector for P if

$$\inf\ (P) = \inf L(\underset{\sim}{X},\ \underset{\sim}{\lambda}^*).$$

The optimality in P may be characterized by the general saddle point condition,

$$\underset{\sim}{\lambda}^* \ \varepsilon\ E^m_+$$

$$\min_{\underset{\sim}{X}\varepsilon L} \ L(\underset{\sim}{X},\ \underset{\sim}{\lambda}^*) = L(\underset{\sim}{X}^*,\ \underset{\sim}{\lambda}^*) = \max_{\underset{\sim}{\lambda}\varepsilon E^m} \ L(\underset{\sim}{X}^*,\ \underset{\sim}{\lambda}).$$

15.2 The Dual Problem and Duality Gap

The dual problem is defined as

$$D:\ \text{Maximize } v(\underset{\sim}{\lambda}),\ \underset{\sim}{\lambda}\ \varepsilon\ E^m$$

$$v(\underset{\sim}{\lambda}) = \inf_{\underset{\sim}{X}\varepsilon L} \ L(\underset{\sim}{X},\ \underset{\sim}{\lambda})$$

The optimal value of the dual is

$$\sup\ (D) = \sup_{\underset{\sim}{\lambda}\varepsilon\ {}^m} \ \inf_{\underset{\sim}{X}\varepsilon L} \ L(\underset{\sim}{X},\ \underset{\sim}{\lambda}).$$

Since min (P) = $\inf\limits_{\underset{\sim}{X}\varepsilon L} \ \sup\limits_{\underset{\sim}{\lambda}\varepsilon E^m} \ L(\underset{\sim}{X},\ \underset{\sim}{\lambda})$, min (P) $\geqq$ sup (D) or in general, inf (P) $\geqq$ sup (D). If inf (P) > sup (D), a duality gap is said to exist between the primal problem P and the dual problem D. If there exists a $\underset{\sim}{\lambda}$ at which the maximum in D is attained, then sup (D) = max (D). If $\underset{\sim}{\lambda}^*$ solves D and min (P) = max (D), then $\underset{\sim}{\lambda}^*$ is a Kuhn-Tucker vector of P.

15.3 Global Optimality and Primal-Dual Method

The necessary condition for optimality may be expressed as follows.

If $\underset{\sim}{X}^*$ is a global minimum of P and min (P) = max (D), then the above saddle point condition holds. The sufficient condition may be reformulated as follows. If $\underset{\sim}{X}^*$ satisfies the above saddle point condition, then it is a global min of P and min (P) - max (D). Further the vector $\underset{\sim}{\lambda}^*$ in the saddle point relation is a global maximizer of D. This vector $\underset{\sim}{\lambda}^*$ is a Kuhn-Tucker vector for P.

The saddle point condition is always sufficient condition for optimality. However it is a necessary condition that is required to establish the duality relation min (P) = max (D). This duality relation is equivalent to the existence of a Kuhn-Tucker vector $\underset{\sim}{\lambda}^*$ of P. The primal-dual methods exploit this duality relation to solve the associated nonlinear problem. In the ideal case, the dual function $v(\underset{\sim}{\lambda})$ may be maximized to get $\underset{\sim}{\lambda}^*$ and then $L(\underset{\sim}{X}, \underset{\sim}{\lambda}^*)$ may be minimized to get $\underset{\sim}{X}^*$. This method of solving P is possible only for some simple problems. The numerical algorithms based on the duality relationship generate a maximizing sequence $\{\underset{\sim}{\lambda}^{(k)}\}$ for D and for each $\underset{\sim}{\lambda}^{(k)}$, generate $\underset{\sim}{X}^{(k)}$ as a solution to min $L(\underset{\sim}{X}, \underset{\sim}{\lambda}^{(k)})$. The sequences are generated so that $\underset{\sim}{\lambda}^{(k)} \to \underset{\sim}{\lambda}^*$ and $\underset{\sim}{X}^{(k)} \to \underset{\sim}{X}^*$. The saddle-point condition may be used to design primal-dual numerical algorithms for solving P only if the duality relationship min (P) = max (D) holds. The satisfaction of this duality relationship depends on the nature of problem functions and the form of the Lagrangian function $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ associated with P.

15.4 Convex Duality

If P is a convex program then the compactness assumption is fulfilled when the set

$$\{\underset{\sim}{X}: \ \underset{\sim}{X} \in L, \ C(\underset{\sim}{X}) > 0\}$$

is compact and nonnull. The duality theory for convex programs has been reviewed in detail by Geoffrion (G1) and Rockafellar (R12), (R13). For a convex program a Kuhn-Tucker vector $\underset{\sim}{\lambda}^*$ ususally exists and the saddle-point condition is always sufficient for the optimality of P at $\underset{\sim}{X}^*$. Rockafellar (R13) established that for a convex program P, min (P) = sup (D) (R13). The point $(\underset{\sim}{X}^*, \underset{\sim}{\lambda}^*)$ is a saddle-point of $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ on $\mathcal{L} \times E^m$, if and only if $\underset{\sim}{X}^*$ solves P and $\underset{\sim}{\lambda}^*$ solves D. If $\underset{\sim}{\lambda}^*$ solves D, then for $\underset{\sim}{X}^*$ to solve P it is necessary and sufficient that (R13)

(i) $\underset{\sim}{X}^*$ minimizes $L(\underset{\sim}{X}, \underset{\sim}{\lambda}^*)$ on $\underset{\sim}{X} \varepsilon \mathcal{L}$

(ii) $c_i(\underset{\sim}{X}^*) \geqq 0$, $\lambda_i^* > 0$ for $c_i(\underset{\sim}{X}^*) = 0$.

Geoffrion (G1) and Lasden (L1) presented the computational applications of the duality theory for convex programs. Several other possible "duals" of P have been proposed using the Lagrangian function $L(\underset{\sim}{X}, \underset{\sim}{\lambda}) = f(\underset{\sim}{X}) - \underset{\sim}{\lambda}^T \underset{\sim}{C}(\underset{\sim}{X})$, $\underset{\sim}{\lambda} \varepsilon E_+^m$. The following dual formulations are reviewed and compared by Geoffrion (G1).

(i) Geoffrion dual G

$$G:\ \underset{\underset{\sim}{\lambda} \varepsilon E_+^m}{\text{Maximize}} \ \{ \inf_{\underset{\sim}{X} \varepsilon \mathcal{L}} \ (f(\underset{\sim}{X}) - \underset{\sim}{\lambda}^T \underset{\sim}{C}(\underset{\sim}{X}))\}$$

(ii) Wolfe dual W

$$W:\ \text{Maximize} \ \ f(\underset{\sim}{X}) - \underset{\sim}{\lambda}^T \underset{\sim}{C}(\underset{\sim}{X})$$

$$\underset{\sim}{\lambda} \geqq 0$$

$$\underset{\sim}{X} \varepsilon \mathcal{L} \subseteq E^n$$

$$\underset{\sim}{\nabla} f(\underset{\sim}{X}) - \sum_i \lambda_i \underset{\sim}{\nabla} c_i = 0$$

(iii) Stoer, Mangasarian and Ponstein dual

$$\text{SMP:}\quad \underset{\underset{\sim}{\lambda} \geqq 0}{\text{Maximize}}\quad f(\underset{\sim}{X}) - \underset{\sim}{\lambda}^T \underset{\sim}{C}(\underset{\sim}{X})$$

Subject to

$\underset{\sim}{X}$ minimize $f(\underset{\sim}{X}) - \underset{\sim}{\lambda}^T \underset{\sim}{C}(\underset{\sim}{X})$ over L.

15.5 Duality in Nonconvex Programs

The dual formulation D of P is based on $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ and has inherent limitations (R13). The implicit feasible set in D is

$$\{\underset{\sim}{\lambda}: \ \underset{\sim}{\lambda} \in E_+^m, \quad v(\underset{\sim}{\lambda}) > -\infty\}$$

and it is difficult to determine a representation of this set. This implies that it is difficult to determine whether the inf $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ over $\underset{\sim}{X} \in L$ is finite and attained. Further even if $\underset{\sim}{X}^*$ minimizes $L(\underset{\sim}{X}, \underset{\sim}{\lambda}^*)$ and $\underset{\sim}{\lambda}^*$ solves D, $\underset{\sim}{X}^*$ may not solve P unless there is only one solution to P. The dual formulation D is meaningful only in the convex case, since only in this case it is possible to establish the relation min (P) = sup (D) (R13).

Rockafellar (R12), (R13) and Mangasarian (M2) showed that by associating a different Lagrangian with P, the duality gap in nonconvex programs may be eliminated. A wide variety of Lagrangians may be associated with P and each choice corresponds to a different dual problem. Even though great flexibility is afforded by the theory in the choice of the Lagrangian for P, not all of these are of practical value in computation. The Rockafellar's augmented Lagrangian $\Psi(\underset{\sim}{X}, \underset{\sim}{\lambda}, \underset{\sim}{\sigma})$ is a member of a wide class of Lagrangians and has proved to be useful to developing primal-dual numerical algorithms for solving P. The duality theory in terms of $\Psi(\underset{\sim}{X}, \underset{\sim}{\lambda}, \underset{\sim}{\sigma})$ for nonconvex programs is reviewed in Chapter 3. Detailed analysis of the duality theory based on $\Psi(\underset{\sim}{X}, \underset{\sim}{\lambda}, \underset{\sim}{\sigma})$ may be found in (R6), (R12) and (R13). The duality theory based on $\Psi(\underset{\sim}{X}, \underset{\sim}{\lambda}, \underset{\sim}{\sigma})$ for convex programs was investigated by Rockafellar (R4), (R5).

15.6 Partial Duality

It is not necessary to include the Lagrange multipliers of all the constraints of a problem in the definition of the dual function (G1), (L5). The duality can be defined with respect to any subset of the constraints. If a constraint is used to define the Lagrangian associated with P, it has a dual variable of its own. If a constraint is assigned to define the set L, it will not possess a dual variable. Consider the convex problem P with the constraints partitioned so that the dual is defined with respect to the constraints belonging to the index set J. Let ρ be the number of indices in J. Then the partial dual of P in terms of $L(\underset{\sim}{X}, \underset{\sim}{\lambda})$ and with respect to the set J may be represented as

$$\text{PD:} \quad \text{maximize } v(\underset{\sim}{\lambda}), \quad \underset{\sim}{\lambda} \in E^{p}$$

$$v(\underset{\sim}{\lambda}) = \inf_{\underset{\sim}{X}} L(\underset{\sim}{X}, \underset{\sim}{\lambda}) \quad \underset{\sim}{X} \in L, \quad \underset{\sim}{\lambda} \in E^{p}$$

$$c_i(\underset{\sim}{X}) \geqq 0 \qquad i \notin J.$$

The choice of assignment of a constraint depends on the structure of the problem, or the nature of the theoretical analysis or the ease of evaluating $v(\underset{\sim}{\lambda})$.

APPENDIX B

COMPUTERIZED ALAG ALGORITHM AND APPLICATION

1. Introduction

An ALAG penalty function algorithm to solve the equality and inequality constrained problem P3 (see Chapter 3) is presented. An equality constrained problem and an inequality constrained problem are solved using this numerical algorithm. The algorithm and the examples supplement the review of the ALAG penalty function technique reviewed within this report. This numerical algorithm was investigated by Fletcher (F8). This algorithm incorporates the parameter iterations that have been proven to be efficient (F8). A Quasi-Newton method that utilizes a complimentary Davidson-Fletcher-Powell update [F4] for solving unconstrained problems is used in the inner iterations,

2. ALAG Penalty Function Algorithm for Equality and Inequality Constrained Problem.

The equality and inequality constrained problem P3 is defined in section 3.4.1. To simplify the presentation of the numerical algorithm in the next section, following notations are used.

E : The index set of equalities

$$E = \{ i : 1 \leqq i \leqq k \}$$

Sc_i : The scale factor for ith constraint

$WW_i^{(k)}$: The scaled constraint violation for ith constraint in iteration k

$$WW_i^{(k)} = \frac{\left|(C_i^{(k)})\right|}{Sc_i} \begin{cases} i \; E \; E \\ i \notin E \text{ and } C_i^{(k)} < O_i^{(k)} \end{cases}$$

$$WW_i^{(k)} = \frac{\left|\min(C_i^{(k)}, 0)\right|}{Sc_i} \quad i \notin E \text{ and } C_i^{(k)} \geqq \theta_i^{(k)}$$

$AKK^{(k)}$: The largest scaled constraint violation in iteration k

$$AKK^{(k)} = \max_i \left\{ WW_i^{(k)} \right\}$$

$AK^{(k)}$: Initial value of $AKK^{(k)}$ in iteration k

AKMIN : The relative error tolerance required in the constraint residuals c_i. When $AKK^{(k)} \leqq$ AKMIN the algorithm is terminated. This is the stopping criterion for the outer iteration.

EPS_i The tolerance in x_i for unconstrained minimization

$c_i^{(k)}$: The current value or residual of ith constraint in iteration k.

$M(\underset{\sim}{\lambda}^{(k)})$: The index set of constraints that contribute to the ALAG penalty function. $M(\underset{\sim}{\lambda}^{(k)}) = \left\{ i : \; i \varepsilon E \text{ or } i \notin E \text{ and } c_i^{(k)} < \theta_i^{(k)} \right\}$

p : The number of indices in $M(\underset{\sim}{\lambda}^{(k)})$.

$(\Delta\lambda_i)_{PH}^{(k)}$: The Powell-Hestenes correction for $\lambda_i^{(k)}$ in kth iteration

$(\Delta\lambda_i)_N^{(k)}$: The Newton correction for $\lambda_i^{(k)}$ in kth iteration.

Algorithm A3

(i) Select

the initial starting point $\underset{\sim}{X}^{(0)}$,

the initial estimate of parameter vector $\underset{\sim}{\theta}^{(1)}$

the initial penalty constants $\sigma_i^{(1)}$, $\forall$ i

(ii) $k = k + 1$

(iii) Minimize $\Phi\ (\underset{\sim}{X}, \underset{\sim}{\theta}^{(k)}, \underset{\sim}{\sigma}^{(k)})$ to find

$\underset{\sim}{X}^{(k)} = \underset{\sim}{X}\ (\underset{\sim}{\theta}^{(k)}, \underset{\sim}{\sigma}^{(k)})$, starting the unconstrained

minimization from $\underset{\sim}{X}^{(k-1)}$.

- Use Broyden's Quasi-Newton method for unconstrained minimization of $\Phi\ (\underset{\sim}{X}, \underset{\sim}{\theta}^{(k)}, \underset{\sim}{\sigma}^{(k)})$

$$\Phi\ (\underset{\sim}{X}, \underset{\sim}{\theta}^{(k)}, \underset{\sim}{\sigma}^{(k)}) = f(\underset{\sim}{X}) + 1/2 \sum_{i\varepsilon E} \sigma_i^{(k)} [C_i - \theta_i^{(k)}]^2 + \frac{1}{2} \sum_{i \notin E} \sigma_i^{(k)} (C_i - \theta_i^{(k)})_-^2$$

$$(C_i - \theta_i)_- = \begin{cases} 0, & C_i - \theta_i \geqq 0 \\ (C_i - \theta_i), & C_i - \theta_i < 0 \end{cases}$$

During the unconstrained minimization of Φ, an estimate of the Hessian of Φ is built-up using the first order information about $f\ (\underset{\sim}{X})$, $c_i\ (\underset{\sim}{X})$ and the change in $\underset{\sim}{X}$. The estimate of the Hessian of Φ at $(\underset{\sim}{X}^{(k)}, \underset{\sim}{\theta}^{(k)}, \underset{\sim}{\sigma}^{(k)})$ is represented as $G(\underset{\sim}{\sigma}^{(k)})$.

(iv) Estimate

the Lagrange multiplier estimates $\lambda_i^{(k)} = \sigma_i^{(k)}\ \theta_i^{(k)}$

the constraint residuals $c_i^{(k)}$,

the scaled constraint violations $WW_i^{(k)}$,

the largest scaled constraint violation $AKK^{(k)}$.

If $AKK^{(k)} \leqq AKMIN$, stop.

If $AKK^{(k)} \geqq AK^{(k)}$ go to (viii). Otherwise go to (v).

(v) Estimate $(\Delta\lambda_i)_{PH}^{(k)}$

$$(\Delta\lambda_i)_{PH}^{(k)} = -\ \sigma_i^{(k)}\ C_i^{(k)} \quad i\varepsilon E \text{ or}$$

$$i \notin E \quad \lambda_i \neq 0,\ C_i < 0,\ \lambda_i^{(k)} - \sigma_i^{(k)}\ C_i^{(k)} \geqq 0$$

$$(\Delta\lambda_i)_{PH}^{(k)} = -\ \lambda_i^{(k)} \quad i \notin E,\ \lambda_i \neq 0,\ C_i < 0,$$

$$\lambda_i^{(k)} - \sigma_i^{(k)}\ C_i^{(k)} < 0$$

the constraint tolerance AKMIN

the tolerance EPS_i on variable x_i

the constraint scale factors Sc_i

the initial upper bound on constraint violation $AK^{(1)}$

$k = 0$

If $k = 1$, go to (vi).

If $\left| X_i^{(k)} - x_i^{(k-1)} \right| \leqq EPS_i$, stop.

Otherwise go to (vi).

(vi) Find $R = \left\{ i \; : \; i \varepsilon E \text{ or } i \notin E \text{ and } \lambda_i \neq 0 \text{ and } c_i^{(k)} < 0 \right\}$

Let p be the number of indices in R and

$$\underset{\sim}{Y}^{(k)} = (Y_1^{(k)}, Y_2^{(k)}, \ldots, Y_p^{(k)})^T \; \varepsilon \; E^p$$

Estimate $Y_i^{(k)} = (\Delta\lambda_i)_N^{(k)}$, $i \varepsilon R$.

The $Y_i^{(k)}$, $i \varepsilon R$ are determined by solving the following subproblem.

Min $Q(Y_i^{(k)})$

$$Y_i^{(k)} \geqq - \lambda_i^{(k)}, \; i \varepsilon R$$

$$Q(Y_i^{(k)}) = \sum_{i\varepsilon R} C_i Y_i^{(k)} + \frac{1}{2} \underset{\sim}{Y}^{(k)^T} (N^T G_1^{-1} N) \underset{\sim}{Y}^{(k)}$$

where G is the estimate of the Hessian of Φ and the columns of N are the gradients of c_i, $i \varepsilon R$.

(vii) $\lambda_i^{(k+1)} = \lambda_i^{(k)} + Y_i^{(k)} \quad i \in R.$

$$Z_i^{(k)} = 4\left|\frac{(\Delta\lambda_i)_{PH}^{(k)} - (\Delta\lambda_i)_{N}^{(k)}}{(\Delta\lambda_i)_{PH}^{(k)}}\right|$$

If $Z_i(k) > 1$, $\sigma_i^{(k+1)} = Z_i^{(k)}\ \sigma_i^{(k)}$ and $d_i^{(k)} = (Z_i^{(k)} - 1)\sigma_i^{(k)}$, $i \in R$.

If $Z_i^{(k)} \leqq 1$, $\sigma_i^{(k+1)} = \sigma_i^{(k)}$ and $d_i^{(k)} = 0$, $i \in R$.

$G(\underset{\sim}{\sigma}^{(k+1)}) = G(\underset{\sim}{\sigma}^{(k)}) + N\ D^{(k)} N^T$

$D^{(k)} = \text{diag}\ (d_1^{(k)}, d_2^{(k)}, \ldots., d_p^{(k)}).$

$AK^{(k)} = AKK^{(k)}$

go to (ix).

(viii) Find $D = \left\{ i \ : \ WW_i^{(k)} > AK^{(k)} \text{ or } WW_i^{(k-1)} < 4\ WW_i^{(k)} \right\}$

Set $\sigma_i^{(k+1)} = 10\ \sigma_i^{(k)}$ and $\lambda_i^{(k+1)} = \lambda_i^{(k)}$

The change in $\sigma_i^{(k)}$ is $d_i^{(k)} = 9\ \sigma_i^{(k)}$, $i \in D$, and $d_i^{(k)} = 0$, $i \notin D$. Let $D^{(k)}$ be the diagonal matrix with $d_i^{(k)}$ as elements. The estimate $G(\underset{\sim}{\sigma}^{(k)})$ of the Hessian of Φ is adjusted to account for the change in $\underset{\sim}{\sigma}^{(k)}$ as follows.

$G(\underset{\sim}{\sigma}^{(k+1)}) = G(\underset{\sim}{\sigma}^{(k)}) + N^{(k)}\ D^{(k)}\ N^{(k)T}$

The columns of $N^{(k)}$ are the gradients of constraints whose indices are in D

If $\left| x_i^{(k)} - x_i^{(k-1)} \right| \leqq EPS_i$, stop.

Otherwise go to (ix).

(ix) $\theta_i^{(k+1)} = \lambda_i^{(k+1)} / \sigma_i^{(k+1)} \quad \forall_i$

go to (ii).

3. Numerical Examples

3.1. Example 1: Equality constrained Problem

Minimize : $f\ (\underset{\sim}{X}) = (x_1 - 1)^2 + (x_1 - x_2)^2 + (x_2 - x_3)^2 + (x_3 - x_4)^4 + (x_4 - x_5)^4$

Subject to $c_1\ (\underset{\sim}{X}) = x_1 + x_2^2 + x_3^3 - 2 - 3\sqrt{2} = 0$

$c_2\ (\underset{\sim}{X}) = x_2 - x_3^2 + x_4 + 2 - 2\sqrt{2} = 0$

$c_3\ (\underset{\sim}{X}) = x_1 x_5 - 2 = 0$

Starting point $\underset{\sim}{X}^{(0)} = (2,2,2,2,2)$

Solution point $\underset{\sim}{X}^* = (1.1911,\ 1.3626,\ 1.4728,\ 1.635,\ 1.679)$

Optimal objective function value $f^* = 7.8776 \text{ X } 10^{-2}$.

The relative error tolerance in constraint residuals AKMIN = 0.0008

The error tolerance in variables $EPS_i = 0.00001 \ \forall\ i$

Outer Iteration 1

$\underset{\sim}{X}^{0} = (2,2,2,2,2)$

$\underset{\sim}{\theta}^{(1)} = (0,0,0)$.

$S\underset{\sim}{C} = (7.75736,\ 1.0,\ 2.0)$

$\underset{\sim}{\sigma}^{(1)} = (0.03323,\ 2.0,\ 0.5)$

$AK^{(1)} = 10 \text{ X } 10^{60}$

Inner iteration

$\underset{\sim}{X}^{(1)} = (1.15955,\ 1.28716,\ 1.38550,\ 1.46505,\ 1.70426)$

$\underset{\sim}{C}^{(1)} = (-.76667,\ 0.00417,\ -0.023827)$

$W\underset{\sim}{W}^{(1)} = (0.09883,\ 0.00417,\ 0.01191)$

$AKK^{(1)} = 0.09883$

Updating of parameters

3 Active Constraints $i = 1,2,3$

$\Delta\underset{\sim}{\lambda}^{(1)} = (0.08186,\ -\ 0.06302,\ -.12599)$, $\underset{\sim}{\lambda}^{(1)} = 0$

$\sigma_1^{(1)}$ increased to 0.29414

$\sigma_2^{(1)}$ increased to 52.44928

$\sigma_3^{(1)}$ increased to 23.15088

Outer Iteration 2

$\underset{\sim}{X}^{(1)} = (1.15955, 1.28716, 1.38550, 1.46505, 1.70426)$

$\underset{\sim}{\theta}^{(2)} = (.27830, -.00120, -.00544)$

$\underset{\sim}{\sigma}^{(2)} = (0.29414, 52.44928, 23.15088)$

$AK^{(2)} = 0.09883$

Inner iteration

$\underset{\sim}{X}^{(2)} = (1.19807, 1.37601, 1.48774, 1.66416, 1.66479)$

$\underset{\sim}{C}^{(2)} = (0.14175, -.00162, -0.00546)$

$W\underset{\sim}{W}^{(2)} = (0.01827, 0.00162, 0.00273)$

$AKK^{(2)} = 0.01827$

Updating of parameters

$\underset{\sim}{\lambda}^{(2)} = (0.08186, -0.06302, -0.12599)$

$\Delta\underset{\sim}{\lambda}^{(2)} = (-0.04160, 0.06244, 0.10922)$

3 active constraints $i = 1,2,3$.

$\sigma_2^{(2)}$ increased to 55.921

Outer Iteration 3

$\underset{\sim}{X}^{(2)} = (1.19807, 1.37601, 1.48774, 1.66416, 1.66479)$

$\underset{\sim}{\theta}^{(3)} = (.13687, -0.00001, -0.00072)$

$\underset{\sim}{\sigma}^{(3)} = (0.29414, 55.921, 23.1509)$

$AK^{(3)} = 0.01827$

Inner iteration

$\underset{\sim}{X}^{(3)} = (1.1914, 1.36313, 1.47324, 1.63544, 1.67807)$

$\underset{\sim}{C}^{(3)} = (0.00452, -0.00031, -0.00074)$

$W\underset{\sim}{W}^{(3)} = (0.00058, 0.00031, 0.00037)$, $AKK^{(3)} = 0.00058$

$f\ (\underset{\sim}{X}^{(3)}) = 0.07895.$

This is the optimal solution for specified stopping criterion

AKMIN = 0.0008.

3.2 Example 2: Inequality constrained problem

Minimize $f\ (\underset{\sim}{X}) = 2 - \frac{1}{120}\ (x_1 x_2 x_3 x_4 x_5)$

Subject to $c_i\ (X) = x_i \geqq 0\ i = 1,2,\ldots.,5$

$c_{i+5}\ (X) = i - x_i \geq 0\ i = 1,2,\ldots.,5$

Starting point $\underset{\sim}{X}^0 = (2,2,2,2,2)$

Solution point $\underset{\sim}{X}^* = (1,2,3,4,5)$

Optimal objective function value $f^* = 1.0.$

The relative error tolerance in constraint residuals AKMIN = 0.0008

The error tolerance in variables $EPS_i = 0.0001$

Outer Iteration 1

$\underset{\sim}{X}^{0} = (2,2,2,2,2)$

$\underset{\sim}{\theta}^{(1)} = 0$

$Sc_{i} = 1.0 \ \forall \ i$

$\sigma^{(1)} = 3.46667 \ \forall \ i$

$AK^{(1)} = 10 \text{ X } 10^{60}$

Inner iteration

$\underset{\sim}{X}^{(1)} = (1.35159, 2.21458, 3.15082, 4.11547, 5.0933)$

$\underset{\sim}{WW}^{(1)} = (0,0,0,0,0,0,35159, .21458, .15082, .11547, .0933)$

$AKK^{(1)} = .35159$

Updating of parameters

5 Active constraints i = 6,7,8,9,10.

$\Delta\underset{\sim}{\lambda}^{(1)} = (0,0,0,0,0, .99039, .4847412, .3084211, .2188432, .1978085)$

$\sigma_{7}^{(1)}$ increased to 4.83063

$\sigma_{8}^{(1)}$ increased to 5.6865

$\sigma_{9}^{(1)}$ increased to 6.2857

$\sigma_{10}^{(1)}$ increased to 5.3862

Outer Iteration 2

$\underset{\sim}{x}^{(1)} = (1.35159, 2.21458, 3.15082, 4.11547, 5.0933)$

$\underset{\sim}{\theta}^{(2)} = (0,0,0,0,0, .28569, 0.10035, 0.05424, 0.03482, 0.03673)$

$\underset{\sim}{\sigma}^{(2)} = (3.46667, 3.46667, 3.46667, 3.46667, 3.46667, 3.46667,$
$4.8306, 5.68664, 6.28569, 5.3862)$

$AK^{(2)} = 0.35159$

Inner iteration

$\underset{\sim}{x}^{(2)} = (1.00438, 2.004, 3.0049, 4.0054, 5.00085)$

$\underset{\sim}{WW}^{(2)} = (0,0,0,0,0, 0.00438, 0.00395, 0.00486, 0.005399, 0.000854)$

$AKK^{(2)} = 0.00539$

Updating of parameters

$\underset{\sim}{\lambda}^{(2)} = (0,0,0,0,0, 0.99039, 0.48474, 0.308421, 0.21884, 0.197808)$

$\Delta\underset{\sim}{\lambda}^{(2)} = (0,0,0,0,0, 0.01006, 0.01533, 0.025028, 0.031898, 0.00273)$

5 active constraints $i = 6,7,8,9,10$

$\sigma_6^{(2)}$ increased to 4.68405

$\sigma_{10}^{(2)}$ increased to 8.76983

Outer Iteration 3

$\underset{\sim}{x}^{(2)} = (1.0043, 2.0039, 3.0049, 4.0054, 5.0009)$

$\underset{\sim}{\theta}^{(3)}$ = (0,0,0,0,0, 0.2136, 0.1035, 0.05864, 0.03989, 0.02287)

$\underset{\sim}{\sigma}^{(3)}$ = (3.46667, 3.46667, 3.46667, 3.46667, 3.46667,
4.68405, 4.8306, 5.6866, 6.2857, 8.7698)

$AK^{(3)}$ = 0.00540

Inner iteration

$\underset{\sim}{X}^{(3)}$ = (1,2,3,4,5)

$\underset{\sim}{WW}^{(3)}$ = (0,0,0,0,0, 0.00011, 0.000031, 0.000031, 0.00013, 0.000067)

f $(\underset{\sim}{X}^{(3)})$ = 1.00018, $AKK^{(3)}$ = 0.00013

This is the optimal solution for specified stopping criterion

AKMIN = 0.0008.

APPENDIX C

COMPUTER PROGRAM DOCUMENTATION

This particular section of the report contains the pertinent documentation for the computer programs designed and implemented in conjunction with this research grant. Three different computer programs were developed all based upon the Augmented Lagrangian Penalty Function technique for Nonlinear Programming. These programs differ from each other primarily as a function of the type of unconstrained optimizer used. These programs are entitled ALAG1 through ALAG3. ALAG1 and ALAG2 require closed form gradient equations for the functions to be optimized. Whereas ALAG3 does not require gradient information be supplied by the user.

TABLE I. Unconstrained Optimizers for ALAG Computer Programs

Computer Program	Unconstrained Optimizer
ALAG 1	Fletcher algorithm using a quasi-Newton complimentary Davidon-Fletcher-Powell update formula (P4)
ALAG 2	Variable metric method without line searches as proposed and analyzed by Powell (P5)
ALAG 3	Same method as ALAG1 except derivatives are estimated by differences

COMPUTER PROGRAM: ALAG 1

LANGUAGE: FORTRAN

TECHNICAL REFERENCES: (F8), (P4)

ALAG 1

1. PURPOSE: To minimize a function $F(\underline{\bar{x}}) = f(X_1, \ldots, X_n)$ subject to both equality and inequality constraints. Derivatives of all functions must be supplied in a user subroutine entitled ALAGB (see item 5). An initial estimate of the solution (not necessarily feasible) must be specified. This computer program is developed from algorithm of section .

2. USE: CALL ALAG1 (N,M,K,X,EPS, AKMIN, DFN, MAXFN, IPR1, IPR2, IW, MODE)

N An INTEGER set to the number of variables n ($N \geq 2$).

M An INTEGER set to the total number of constraints m ($M \geq 1$).

K An INTEGER set to the total number of equality constraints k.

X A REAL array of N elements in which the initial estimate of the solution must be set. ALAG1 returns the solution $\bar{x}$ in X.

EPS A REAL array of N elements, in which the tolerances for the unconstrained minimizations must be set. EPS (I) should be set so that EPS (I)/X (I) = AKMIN, roughly speaking.

AKMIN A REAL number in which the relative error tolerance required in the constraint residuals must be set. ALAG1 will exit when $\max\{|c_i(x)|/\text{scaling factor for } c_i\} \leq$ AKMIN for the active constraints {i}.

DFN A REAL number in which the likely reaction in $F(\underline{\bar{x}})$ must be set. This is done in the same way as for QNWTA - see the QNWTA description.

MAXFN An INTEGER in which the maximum number of calls of ALAGB on any one unconstrained minimization must be set.

IPR1 An INTEGER controlling the frequency of printing from ALAG1. Printing occurs every IPR1 iterations, except for details of increases to the c_i which are always printed. No printing at all occurs (except for error diagnostics) if IPR1 = 0.

IPR2 An INTEGER controlling the frequency of printing from QNWTA. IPR2 should be set as described in the QNWTA documentation.

IW An INTEGER giving the amount of storage available in COMMON/ALAGL/W(.). Set to 2500 unless wishing to change the restrictions (see Section 5).

MODE An INTEGER controlling the mode of operation of ALAG1. If any positive definite estimate is available of the hessian matrix of the penalty function, set |MODE| = 2 or 3, otherwise set |MODE| = 1 (see QNWTA description). If estimates of the σ_i and Θ_i parameters are available (see item 8) set MODE < 0, otherwise set MODE > 0. A normal setting for a one-off job with no information available is MODE = 1.

3. LABELED COMMON AREAS:

Certain labeled COMMON areas must be declared and set on entry to ALAG1.

COMMON/ALGAGE/C(150) Set scale factors (>0) for the constraints in C(1), C(2),....,C(M). Choose the magnitude of these scale factors to give an indication of the constraints evaluated about the initial approximation $\underline{x}$. If any constraints are violated by an amount greater in modulus than that which is set, then the setting is increased accordingly. These scale factors are transferred to C(M+1), C(M+2),.....,C(2M) by ALAG1.

COMMON/ALAGF/GC(25,50) Set the derivatives of any linear constraints on entry rather than in ALAGB. This is the most efficient and the numbers are not disturbed. The manner of setting is described in item 4.

COMMON/ALAGG/T(150) If MODE < 0 is used, then set the parameters $\Theta_1,\Theta_2, \ldots, \Theta_m$ in T(1), T(2),...,T(M) and the parameters $\sigma_1,\sigma_2, \ldots,\sigma_m$ in T(M+1),T(M+2),...,T(2M). The meaning of these parameters may be found in section of this report.

COMMON/ALAGI/G2P(325) If |MODE| = 2 or 3 set the estimated hessian matrix of the penalty function in G2P(1),..., G2P(N·(N+1)/2). The manner of setting is that described in QNWTA under the heading MODE.

Local storage for ALAG1 is through labeled COMMON areas. These have been set on the assumption that $N \leq 25$ and $M \leq 50$. If it is desired to remove either or both of these restrictions, then it is necessary to increase the storage available in some or all of these areas. This can be done by defining the named COMMON areas in the users MAIN with the increased storage settings, in which case the extra storage will be effective throughout the whole program. The complete list of labeled COMMON used by ALAG1 and the corresponding values of N and M are as follows.

COMMON/ALAGC/F,M,K,IS,MK,NU		independent of N and M
"	D/G(50)	2N
"	E/C(150)	3M
"	F/GC(25,50)	N,M
"	G/T(150)	3M
"	H/GP(50)	μ (μ = max(M,N))
"	I(G2P(325)	N·(N+1)/2
"	J/V(50)	μ
"	K/WW(150)	3μ
"	L/W(2500)	μ^2
"	M/ZZ(100)	2μ
"	N/LT(100)	2M

4. ACCURACY: This iterative algorithm terminates normally when the following convergence condition is met: $\max \{|c_i(x)|/\text{scaling factor for } c_i\} \le$ AKMIN for i an element of the set of active constraint indices. A diagnostic message for abnormal termination is printed when the program is unable to achieve the requested accuracy. This may be due to (i) a mistake in programming ALAGB, (ii) there is no feasible point (in which case $\sigma_i \to \infty$ and $c_i \to$ constant $\neq 0$), (iii) EPS has been set too large relative to AKMIN, (iv) the problem is too ill-conditioned.

OTHER ROUTINES: ALAG1 requires the use of ALAGB, ALAGZ, BQDMA, MULDA, MULDB, MULDE, and QNWTA

ALAGB: USER SUBROUTINE The user must define a subroutine headed by

```
SUBROUTINE ALAGB(N,M,X)
REAL X(1)
COMMON/ALAGC/F
COMMON/ALAGD/G(50)
COMMON/ALAGE/C(150)
COMMON/ALAGF/GC(25,50)
```

This subroutine takes the vector X and sets

(1) $F(\overline{x})$ in F; (2) $c_1(\overline{x}),\ldots, c_m(\overline{x})$ in C(1),...,C(M);

(3) $(\partial F/_{\partial X_1},\ldots,\partial F/_{\partial X_n})|_{\overline{x}}$ in G(1),...,G(N);

(4) $(\partial c_i/_{\partial X_1},\ldots,\partial c_i/_{\partial X_n})|_{\overline{x}}$ in GC(1,I),...

GC (N,I) for I = 1,...,M.

ALAGZ: This subroutine evaluates the augmented function comprised of the original objective function and penalty terms that is to be optimized.

SUBROUTINE ALAGZ (N, X, PHI, GPHI)

N and X as previously defined.

PHI is the value of the augmented function evaluated at X.

GPHI is the gradient of the augmented function evaluated at X.

BQDMA: The purpose of BQDMA is to find the values that minimize a quadratic of n variables subject to upper and lower bounds on some or all of the variables.

The quadratic is defined by

$$Q(X) = 1/2\ X^t\ AX - B^tX$$

Subject to:

$$BL_i \le X_i \le BU_i \qquad i = 1,\ldots,N.$$

SUBROUTINE BQDMA (N,A,IA,B,BL,BU,X,Q,LT,K,G)

N an INTEGER which must be set by the user to the number of variables.

A a REAL, two dimensional array, each dimension at least N; the elements in the upper triangle A(I,J) $I \le J \le N$ must be set by the user to the corresponding A_{ij} in (1), and will remain untouched by the subroutine. Elements A(I,J) $N \ge I > J$ are used as working space.

IA an INTEGER giving the first dimension of A in the statement which assigns space to A.

B a REAL array of at least N elements. The user must set B(I). B is not overwritten by BQDMA.

BL a REAL array of at least N elements. The user must set BL(I) to the lower bound on the I^{th} variable. If the bound is non-existent, set it to a very small number like -1E75. BL is not overwritten by BQDMA.

BU a REAL array of at least N elements. The user must set BU(I) to the upper bound on the I^{th} variable. If the bound is non-existent, set it to a very large number. BU is not overwritten by BQDMA.

X a REAL array of at least N elements. BQDMA returns the solution in X(I).

Q a REAL variable in which BQDMA returns the solution value of the quadratic.

LT an INTEGER array of at least N elements, set by BQDMA to a permutation of the integers 1,2,...,N (see K and G below)

K an INTEGER set by BQDMA to the number of free variables at the solution (those not on their bounds). These are the variables LT(1), LT(2),...,LT(K).

G a REAL array of at least 3*N elements. G(1),....,G(N) are set by BQDMA to the gradient evaluated at the solution point. G is indirectly addressed so that G(I) contains the gradient with respect to the LT(I) variable, whence G(1),....,G(K) will be found to be zero. G(N+1),...,G(3*N) are used by BQDMA as working space.

MULDA is a subroutine for use in problems which involve the addition or subtraction of rank one matrices $\sigma\ \underline{zz}^T$ to positive definite or semi-definite symmetric matrices A stored in factored form $A = LDL^T$, such that the resulting N x N matrix

$$\tilde{A} = A + \sigma\ \underline{zz}^T$$

is also known to be positive definite or semi-definite. Note that L is lower triangular with $\ell_{ii}=1$, and D is diagonal with $d_i \geq 0$.

SUBROUTINE MULDA (A, N, Z, SIG, W, IR, MK, EPS)

A	A REAL one dimensional array of N*(N+1)/2 elements in which the matrix $A=LDL^T$ must be given in factored form. The order in which elements of L and D are stored is $d_1, \ell_{21}, \ell_{31}, \ldots, \ell_{N1}, d_2, \ell_{32}, \ldots, \ell_{N2}, \ldots \ \ldots$ $d_{N-1}, \ell_{N,N-1}, d_N$. The factors of the matrix $\tilde{A} = A + \sigma\ \overline{zz}^T$ will overwrite those of A on exit.

N	An INTEGER ($N\geq 1$) which must be set to the dimension of the problem.

Z	A REAL one dimensional array of N elements in which the vector $\bar{z}$ must be set, The array Z is overwritten by the routine.

SIG	A REAL variable in which the scalar σ must be set. SIG is not restricted to $\underline{+}$., but if SIG<0 then it must be known from other considerations that $\tilde{A}$ is positive definite or semi-definite, apart from the effects of round-off error.

W — A REAL array of N elements. If SIG>0 then W is not used, and the name of any one dimensional array can be inserted in the calling sequence. If SIG<0 then W is used as work space. In addition for SIG<0 it may be possible to save time by setting in W the vector v defined by $L\bar{v}=\bar{z}$. The ways in which this can occur are described under MK below.

IR — An INTEGER to be set so that $|IR|$ is the rank of A. If the rank of $\tilde{A}$ is expected to be different from that of A, set $IR\leq 0$. On exit from MULDA, $IR(\geq 0)$ will contain the rank of $\tilde{A}$.

MK — An INTEGER to be set only when SIG<0, as follows. If the vector $\bar{v}$ defined by $L\bar{v}=\bar{z}$ has not been calculated previously, set MK=0. If MULDA has been used previously to calculate $A^{-1}\bar{z}$, then $\bar{v}$ is a by-product of this calculation and is stored in the W parameter of MULDE. In this case transfer v to the W parameter of MULDA and set MK=1. If $\bar{z}$ has been calculated as $\bar{z} = A\bar{u}$ for some arbitrary vector $\bar{u}$ using MULDD, then again $\bar{v}$ is a by-product of the calculation and is available in the W parameter of MULDD. In this case (or any other in which $\bar{v}$ is known) set $\bar{v}$ in the W parameter of MULDA and set MK=2.

EPS — A REAL variable to be set only when SIG<0 and $\tilde{A}$ is expected to have the same rank as A. In certain ill-conditioned cases a non-zero diagonal element of $\tilde{D}$ might become so small as to be indeterminate. Two courses of action are possible. One is to introduce a small perturbation in order that $\tilde{A}$ keeps the same rank as A. This is the normal course of action and is achieved by setting EPS equal to the relative machine precision ε. The other course of action is to let the rank of $\tilde{A}$ be one less than the rank of A. This is achieved by setting EPS equal zero.

MULDB - factorizes a positive definite symmetric matrix given in A. This matrix is then used in MULDA.

SUBROUTINE MULDB (A, N, IR)

A Must contain the elements of A in the order $a_{11},a_{21},\ldots,a_{N1},a_{22},a_{32},\ldots a_{N2},\ldots,a_{N-1,N-1},a_{N,N-1},a_{NN}$; that is as successive columns of its lower triangle). On exit A will be overwritten by the factors L and D in the form described in MULDA.

N Order of the matrix A,

IR An INTEGER set by MULDB to the rank of the factorization. If the factorization has been performed successfully IR=N will be set. If IR<N then the factorization has failed because A is not positive definite (possibly due to round-off error). In this case the factors of a positive semi-definite matrix

of rank IR will be found in A. However the results of this calculation are unpredictable, and MULDB should not be used in an attempt to factorize positive semi-definite matrices.

MULDE calculates the vector $\bar{z}* = A^{-1}\bar{z}$ where A is in factored form

SUBROUTINE MULDE (A, N, Z, W, IR)

A Must be set in factored form.

N Order of the matrix A.

Z A REAL array of N elements to be set to the vector $\bar{z}$. On exit Z contains the vector $\bar{z}* = A^{-1}\bar{z}$.

W A REAL array of N elements which is set by MULDE to be vector $\bar{v}$ defined by $L\bar{v}=\bar{z}$. If this vector is not of interest, replace W by Z in the calling sequence to obviate the need to supply extra storage.

IR An INTEGER which must be set to the rank of A.

QNWTA finds the minimum of a function $F(\bar{x})$ of several variables given that the gradient vector can be calculated. This routine is based upon a quasi-Newton method described by Fletcher in (F8).

SUBROUTINE QNWTA (FUNCT, N, X, F, G, H, W, DFN, EPS, MODE, MAXFN, IPRINT, IEXIT).

FUNCT An IDENTIFIER of the users subroutine.

N An INTEGER to be set to the number of variables ($N \geq 2$).

X A REAL ARRAY of N elements in which the current estimate of the solution is stored. An initial approximation must be set in X on entry to QNWTA and the best estimate obtained will be returned on exit.

F A REAL number in which the best value of $F(\bar{x})$ corresponding to X above will be returned.

G A REAL ARRAY of N elements in which the gradient vector corresponding to X above will be returned. Not to be set on entry.

H A REAL ARRAY of N*(N+1)/2 elements in which an estimate of the hessian matrix is stored. The matrix is represented in the product form LDL where L is a lower triangular matrix with unit diagonals and D is a diagonal matrix. The lower triangle of L is stored by columns in H excepting that the unit diagonal elements are replaced by the corresponding elements of D. The setting of H on entry is controlled by the parameter MODE.

W A REAL ARRAY of 3*N elements used as working space.

DFN A REAL number which must be set so as to give QNWTA an estimate of the likely reduction to be obtained in F $(\underline{\bar{x}})$. DFN is used only on the first iteration so an order of magnitude estimate will suffice. The information can be provided in different ways depending upon the sign of DFN which should be set in one of the following ways:

DFN>0 the setting of DFN itself will be taken as the likely reduction to be obtained in $F(\bar{x})$.

DFN=0 it will be assumed that an estimate of the minimum value of $F(\bar{x})$ has been set in argument F, and the likely reduction in $F(\bar{x})$ will be computed according to the initial function value.

DFN<0 a multiple $|DFN|$ of the modulus of the initial function value will be taken as an estimate of the likely reduction.

EPS A REAL ARRAY of N elements to be set on entry to the accuracy required in each element of X.

MODE An INTEGER which controls the setting of the initial estimate of the hessian matrix in the parameter H. The following settings of MODE are permitted.

MODE=1 An estimate corresponding to a unit matrix is set in H by QNWTA.

MODE=2 QNWTA assumes that the hessian matrix itself has been set in H by columns of its lower triangle, and the conversion to LDL^T form is carried out by QNWTA. The hessian matrix must be positive definite.

MODE=3 QNWTA assumes that the hessian matrix has been set in H in product form. This is, convenient when using the H matrix from one problem as an initial estimate for another, in which case the contents of H are passed on unchanged.

MAXFN An INTEGER set to the maximum number of calls of FUNCT permitted.

IPRINT An INTEGER controlling printing. Printing occurs every |IPRINT| iterations and also on exit, in the form

Iteration No, No of calls of FUNCT, IEXIT (on exit only).

Function value

X(1),X(2),...,X(N)	8 to a line
G(1),G(2),...,G(N)	8 to a line

The values of X and G can be suppressed on intermediate iterations by setting IPRINT<0. All intermediate printing can be suppressed by setting IPRINT=MAXFN+1. All printing can be suppressed by setting IPRINT=0.

IEXIT An INTEGER giving the reason for exit from QNWTA. This will be set by QNWTA as follows:

IEXIT=0 (MODE=2 only). The estimate of the hessian matrix is not positive definite.

IEXIT=1 The normal exit in which |DX(1)|<EPS(I) for all I=1,2,...N, where DX(I) is the change in X on an iteration.

IEXIT=2 $G^TDX \geq 0$. Not possible without rounding error. Probable cause is that EPS is set too small for computer word length.

IEXIT=3 FUNCT called MAXFN times.

COMPUTER PROGRAM: ALAG 2

LANGUAGE: FORTRAN

TECHNICAL REFERENCES: (F8), (P5)

The ALAG2 program differs from ALAG1 only in the type of unconstrained optimizer routine employed. Therefore, this section will only document this routine and the user is referred to the documentation on ALAG1 (except for the ALAG1 routine, QNWTA) as being applicable to ALAG2. The unconstrained optimizer routine for ALAG2 is VAMMA. The purpose of VAMM is to calculate the minimum value of a multivariate function. This routine uses the BFGS variable metric method without line searches of the type analyzed by Powell (P5).

SUBROUTINE VAMMA (FUNC, N, X, F, G, SCALE, ACC, W, MAXFN)

FUNC The name of the subroutine provided by the user. It must be declared in an EXTERNAL statement.

N An integer whose value must be set to the number of variables.

X An array of at least n elements, set by the user to initial values of the variables $(x_1,x_2,...,x_n)$. Usually computing time is saved if these estimates are close to the final solution. They are changed automatically to the values that give the least calculated value of the objective function.

F A real variable that is set automatically to the least calculated value of the objective function.

G An array of at least n elements that are set automatically to the components of the first derivative vector of F for the final values of the variables. Small values indicate a successful calculation.

SCALE An array of at least n elements, whose i^{th} component $(1 \leq i \leq n)$ must be set to a positive value that is a suitable change to make to x_i initially in the minimization calculation. About 10% of the total expected change in x_i is often a good value. This array is called SCALE because its elements should reflect the relative sizes of $(x_1, x_2 \ldots, x_n)$.

ACC A real number that defines the required accuracy. The calculation finishes when, for $i=1,2,\ldots,n$. changes in x_i of size ACC*SCALE(i) do not reduce the objective function. When in doubt about the value of ACC it is usually best to choose a small value.

W An array of at least $\frac{1}{2}n(n+13)$ elements that is used as working space. On exit from the subroutine the first $\frac{1}{2}n(n+1)$ locations of W give the final approximation of the second derivative matrix, stored in the factored form used by subroutine MULDA.

MAXFN An INTEGER set to the maximum number of calls of FUNC permitted.

BLOCK COMMON for VAMMA

COMMON/VAMMA/IPRINT,LP,MAXFUN,MODE,NFUN

The five integers called IPRINT,LP,MAXFUN,MODE and NFUN are present in a common block in order that they can be reached by the user. In most calculations they can be ignored, but sometimes they are useful, their purpose being as follows.

IPRINT — This has a default value of zero, and is unchanged by VAMMA. If IPRINT=0, then no printing occurs except perhaps the diagnostic message mentioned below. Otherwise the value of the objective function is printed every |IPRINT| iterations. If IPRINT>0 the values of X(.) and G(.) are printed also. If IPRINT≠0 the final values of F,X(.) and G(.) are always printed.

LP — This has a default value of 6, and is the stream number for any output from VAMMA.

MAXFUN — This has a default value of zero, in which case it does not influence the calculation. However, if it is positive, then VAMMA finishes automatically when the user subroutine is called MAXFUN times. Normal convergence can occur earlier.

MODE — This has a default value of one, in which case the initial approximation to the second derivative matrix is set automatically to a positive diagonal matrix. However, if a suitable positive definite approximation is known, then it may be passed to VAMMA in the first $\frac{1}{2}n(n+1)$ locations of W by setting MODE=2 or MODE=3. When MODE=2 these elements of W must contain the lower triangle of the Hessian approximation, B say, in the order $B_{11},B_{21},B_{31},\ldots,B_{n1}$, $B_{22},B_{32},\ldots,B_{n2},\ldots,B_{n-1\ n-1},B_{n\ n-1},B_{n\ n}$. When MODE=3 the Hessian approximation must be given in the factored form used by subroutine MULDA, which is also the form used to provide the Hessian approximation in W at the return from VAMMA. A check for positive definiteness is made automatically by VAMMA, and if it fails a diagnostic message is printed. In this case the calculation proceeds as though MODE=1, but the actual value of MODE is not changed.

NFUN — This integer is set by VAMMA to the number of times it calls the user subroutine.

COMPUTER PROGRAM: ALAG3

LANGUAGE: FORTRAN

TECHNICAL REFERENCES: (F8)

The ALAG3 program differs from ALAG1 and ALAG2 in the type of unconstrained optimizer routine employed. Therefore, this section will only document this routine and the user is referred to the documentation on ALAG1 as being applicable to ALAG3. The unconstrained optimizer routine employed within ALAG3 is referred to as FDQNW. The purpose of FDQNW is to calculate the minimum value of a multivariate function. The method used is the quasi-Newton method of ALAG1 in which derivatives are estimated by finite difference techniques.

SUBROUTINE FDQNW (FUNCT, N, X, F, G, H, W, DFN, XM, HH, EPS, MODE, MAXFN, IPRINT, IEXIT)

FUNCT — The name of the subroutine provided by the user. It must be declared in an EXTERNAL statement.

N — An INTEGER to be set to the number of variables ($N \geq 2$).

X — A REAL ARRAY of N elements in which the current estimate of the solution is stored. An initial approximation must be set in X on entry to FNQNW and the best estimate obtained will be returned on exit.

F — A REAL number in which the best value of $F(\overline{x})$ corresponding to X above will be returned.

G — A REAL ARRAY of N elements which is used to store an estimate of the gradient vector $\nabla F(\overline{x})$. Not to be set on entry.

H A REAL ARRAY of N*(N+1)/2 elements in which an estimate of the hessian matrix $\partial^2 F/(\partial x_i \partial x_j)$ is stored. The matrix is represented in the product form LDL^T where L is a lower triangular matrix with unit diagonals and D is a diagonal matrix. The lower triangle of L is stored by columns in H excepting that the unit diagonal elements are replaced by the corresponding elements of D. The setting of H on entry is controlled by the parameter MODE.

W A REAL ARRAY of 3*N elements used as working space.

DFN A REAL number which must be set so as to give FDQNW an estimate of the likely reduction to be obtained in $F(\bar{x})$. DFN is used only on the first iteration so an order of magnitude estimate will suffice. The information can be provided in different ways depending upon the sign of DFN which should be set in one of the following ways:

DFN>0 the setting of DFN itself will be taken as the likely reduction to be obtained in $F(\bar{x})$.

DFN=0 it will be assumed that an estimate of the minimum value of $F(\bar{x})$ has been set in argument F, and the likely reduction in $F(\bar{x})$ will be computed according to the initial function value.

DFN<0 a multiple |DFN| of the modulus of the initial function value will be taken as an estimate of the likely reduction.

XM A REAL ARRAY of N elements to be set on entry so that XM(I) > 0 contains an indication of the magnitude of X(I). This quantity need not be set precisely as it is merely used in scaling the problem.

HH A REAL number to be set so that HH*XM(I) contains a step length to be used in calculating G(I) by differences. Set HH equal to $2^{-t/2}$ where t is the number of significant binary digits in the calculation of F.

EPS A REAL number to be set on entry so that the accuracy required in X(I) is EPS*XM(I) for all I, (EPS > 0).

MODE An INTEGER which controls the setting of the initial estimate of the hessian matrix in the parameter H. The following settings of MODE are permitted.

MODE=1 An estimate corresponding to a unit matrix is set in H by FDQNW.

MODE=2 FDQNW assumes that the hessian matrix itself has been set in H by columns of its lower triangle, and the conversion to LDL^T form is carried out by FDQNW. The hessian matrix must be positive definite.

MODE=3 FDQNW assumes that the hessian matrix has been set in H in product form. This is convenient when using the H matrix from one problem as an initial estimate for another, in which case the contents of H are passed on unchanged.

MAXFN An INTEGER set to the maximum number of calls of FUNCT permitted. Up to 2N more calls may be taken if the limit is exceeded whilst evaluating a gradient vector by differences.

IPRINT An INTEGER controlling printing. Printing occurs every |IPRINT| iterations and also on exit, in the form

Iteration No., No of calls of FUNCT, IEXIT (on exit only).
Function value
A(1),X(2),...,X(N)   8 to a line
G(1),G(2),...,G(N)   8 to a line

The values of X and G can be suppressed on intermediate iterations by setting IPRINT<0. All intermediate printing can be suppressed by setting IPRINT=MAXFN+1. All printing can be suppressed by setting IPRINT=0.

IEXIT An INTEGER giving the reason for exit from FDQNW. This will be set by FDQNW as follows:

IEXIT=0 (MODE=2 only). The estimate of the hessian matrix is not positive definite.

IEXIT=1 The normal exit in which $|DX(I)|<EPS(I)$ for all I=1,2,...,N, where DX(I) is the change in X on an iteration.

IEXIT=2 $G^TDX>0$. Either due to rounding errors because EPS is set too small for the computer word length, or to the truncation error in the finite difference formula for G being dominant.

IEXIT=3 FUNCT called MAXFN times.

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