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A NEW APPROACH TO CONSTRAINED FUNCTION OPTIMIZATION.

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A NEW APPROACH TO CONSTRAINED FUNCTION OPTIMIZATION.[†]

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ABSTRACT.

A new approach to the constrained function optimization problem is presented. It is shown that the ordinary Lagrange multiplier method and the penalty function method may be generalized and combined, and the new concept "multiplier function" is introduced. The problem may then be converted into an unconstrained well-conditioned optimization problem. Methods for numerical solution are discussed, and new algorithms are derived.

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1. INTRODUCTION.

In this paper new methods and algorithms for constrained function optimization are presented. The problem considered is minimization of a function f(u) subject to the equality constraint g(u) = 0, where g(u) is an m-dimensional vector with components $g^i(u)$. (The superscript will be used to denote components of a vector. This will simplify the notations later.)

Many methods for solving this problem have been published, but generally they are based on one of two main ideas.

One is the Lagrange multiplier technique, where the constraints are adjoined to the function by means of multipliers λ, to form a new function

$$L(u,\lambda) = f(u) + \sum_{i=1}^{m} \lambda^i g^i(u)$$

generally called the Lagrangian of the problem. The problem is then reduced to finding a saddle-point of $L(u,\lambda)$ in the u-λ space, and thus the dimension of the problem is increased from n to n+m.

The other basic approach is the penalty function method. A function including the constraints in a proper manner is adjoined to the original function f(u), e.g.

$$f(u) + cg^T(u)g(u)$$

where c is a positive real-valued parameter. Under very mild conditions, the solution of

$$\min_u \{f(u) + cg^T(u)g(u)\}$$

tends to the solution of

$$\min_u \{f(u)\}$$

subject to $g(u) = 0$, as c tends to infinity. However, the penalty function method is not very attractive from a numerical point of view, since the functions created become very badly conditioned for numerical optimization. Different ways to overcome this difficulty have been suggested, e.g. by Fiacco and McCormick [1] and by Powell [2]. The basic idea in these papers is to change the penalty function in an iterative way, so as to make the optimum of the penalty function agree with the optimal solution of the problem. However, this requires introduction of a new set of parameters to be iterated on, again increasing the dimension of the minimization problem.

These two basic ideas are combined by Hestenes in [3]. The function

$$F(u,\lambda) = f(u) + \sum_{i=1}^{m} \lambda^i g^i(u) + cg^T(u)g(u)$$

is introduced, and it is shown that for nonsingular problems, $F(u,\lambda^*)$, where λ^* are the optimal multipliers, has a local minimum for $u=u^*$, provided that $c>c_0$. c_0 is a finite real-valued parameter. This is a considerable improvement over both the original Lagrange multiplier technique, and the penalty function methods. The reasons are that c_0 is finite in contrast to the penalty function methods, and that u^* constitutes a minimum of $F(u,\lambda^*)$, while the extremum of $L(u,\lambda^*)$ could have any character. However, it still remains to determine the optimal multipliers λ^*.

The method presented in this paper is a generalization of Hestenes' method. We will introduce the concept "multiplier function", and the m-dimensional vector function $\mu(u)$ is called an admissible multiplier function if it satisfies some simple conditions. The basic condition is that $\mu(u^*) = \lambda^*$. We also define a "generalized Lagrangian" as

$$H(u,c) = f(u) + \mu^T(u)g(u) + cg^T(u)g(u)$$

Using wellknown results, which are briefly stated as lemmas in Section 2, properties of $H(u,c)$ are established in Section 3. It is shown that $H(u,c)$ has an extremum at $u=u^*$, and that there is a finite real-valued c_0, such that $H(u,c)$ for nonsingular problems has an isolated local minimum for $u=u^*$ if $c>c_0$. Properties of $H(u,c)$ for singular problems are also investigated in Section 3.

In Section 4 the multiplier function concept is illustrated with some simple examples. The choice of $\mu(u)$ is discussed, and it is shown that the particular multiplier functions $\mu(u) = \lambda^*$, which is chosen by Hestenes, and $\mu(u) = -\left[g_u(u)g_u^T(u)\right]^{-1}g_u(u)f_u^T(u)$, which has been investigated by Mårtensson [4] and Fletcher [5], may be considered as special cases of this general approach.

Numerical methods for the minimization of $H(u,c)$ are considered in Section 5. Straightforward minimization of the generalized Lagrangian with ordinary function minimization methods, is compared with new algorithms based on properties of the multiplier function $\mu(u)$.

2. NECESSARY AND SUFFICIENT CONDITIONS FOR A CONSTRAINED LOCAL MINIMUM.

In this section we state the necessary and sufficient conditions for a local isolated minimum. For proofs and a more detailed treatment, see e.g. [1], [6].

Introduce the Lagrangian $L(u,\lambda)$ associated with the minimization problem formulated in Section 1.

$$L(u,\lambda) = f(u) + \sum_{i=1}^{m} \lambda^i g^i(u)$$

λ^i are components of the m-dimensional vector λ, generally called the Lagrange multipliers.

We then have

<u>Lemma 1</u> (First order necessary condition)

If

i) f has a local minimum at u^* subject to the constraints $g(u) = 0$,

ii) f and g are once differentiable at u^*,

iii) g_u^i, $i = 1, \ldots, m$, are linearly independent at u^*,

then there exists a unique m-dimensional vector λ^*, such that

$$L_u(u^*,\lambda^*) = 0$$

Notice that i) - iii) are sufficient conditions for the existence of finite Lagrange multipliers λ^*. The constraint qualification iii) may for some problems be replaced by weaker conditions that are sufficient for the existence of λ^*. However, iii) is very useful from a computational point of view, and is assumed to hold in the sequel.

A stronger necessary condition for a minimum is given by the following second-order condition.

<u>Lemma 2</u>

If f and g are twice continuously differentiable at u^*, and if the constraint qualification of Lemma 1 holds at u^*, then a necessary condition for u^* to be a local minimum, is the existence of a vector λ^*, such that

$$g(u^*) = 0$$

$$L_u(u^*,\lambda^*) = 0$$

Further, for every n-dimensional vector y such that $g_u(u^*)y = 0$,

$$y^T L_{uu}(u^*,\lambda^*)y \geq 0$$

This can be strengthened to second-order sufficient conditions.

<u>Lemma 3</u>

Sufficient conditions for u^* to be an isolated local minimum, are that

i) the necessary conditions of Lemma 2 hold,

ii) for every non-zero vector y such that $g_u(u^*)y = 0$,

$$y^T L_{uu}(u^*,\lambda^*)y > 0$$

3. LAGRANGE MULTIPLIER FUNCTIONS.

We now introduce the concept "Lagrange multiplier function".

Definition 1

Let $\mu(u)$ be a real-valued m-dimensional vector defined on R^n. Then $\mu(u)$ is a Lagrange multiplier function for the minimization problem if and only if

i) $\mu(u)$ exists and is twice differentiable in a neighbourhood of u^*,

ii) $\mu(u^*) = \lambda^*$,

iii) for every $y \in R^n$, such that $y \neq 0$, $g_u(u^*)y = 0$, and $y^T L_{uu}(u^*,\lambda^*)y = 0$, $\mu(u)$ satisfies

$$\left\{g_u(u^*)L_{uu}(u^*,\lambda^*) + g_u(u^*)g_u^T(u^*)\mu_u(u^*)\right\}y = 0$$

Condition iii) will prove to be necessary to handle singular problems. In iii) it is also assumed that $f(u)$ and $g(u)$ are at least twice differentiable at $u=u^*$. We assume throughout the paper that this holds in a neighbourhood of u^*.

With the properties of $\mu(u)$ established, we define a "generalized Lagrangian" $H(u,c)$ as follows.

Definition 2

The generalized Lagrangian $H(u,c)$ associated with the minimization problem, is defined as

$$H(u,c) = f(u) + \mu^T(u)g(u) + cg^T(u)g(u)$$

where $\mu(u)$ is an arbitrary multiplier function and c is a real-valued parameter.

With the assumptions made about f(u), g(u) and $\mu(u)$, H(u,c) exists and is twice differentiable in a neighbourhood of u^*.

In the following theorems we will establish some important properties of H.

Theorem 1

For any value of the parameter c, the generalized Lagrangian H(u,c) has a stationary point at $u=u^*$.

Proof: A straightforward differentiation yields

$$H_u = f_u + \mu^T g_u + g^T \mu_u + 2cg^T g_u$$

Since $g(u^*) = 0$, and, according to Lemma 1 and to the definition of $\mu(u)$,

$$f_u(u^*) + \mu^T(u^*)g_u(u^*) = f_u(u^*) + (\lambda^*)^T g_u(u^*) = 0$$

it follows that $H_u(u^*,c) = 0,\ \forall c$

Intuitively it now seems reasonable that the stationary point $u=u^*$ can be made a minimum point by choosing the parameter c large enough. To prove this, we have to distinguish between nonsingular and singular problems.

Theorem 2

Let u^* be a local isolated minimum of $f(u)$ subject to the constraints $g(u) = 0$, and assume that the sufficient conditions of Lemma 3 are satisfied. Then there exists a real-valued parameter c_0, such that $H_u(u^*,c) = 0$ and $H_{uu}(u^*,c) > 0$ for $c>c_0$.

Proof: In Theorem 1 it was shown that $H_u(u^*,c) = 0$ independent of c. Then consider $H_{uu}(u,c)$.

$$H_{uu}(u,c) = f_{uu} + \sum_{i=1}^{m} \mu^i g^i_{uu} + \mu_u^T g_u + g_u^T \mu_u +$$

$$+ \sum_{i=1}^{m} g^i \mu^i_{uu} + 2cg_u^T g_u + 2c \sum_{i=1}^{m} g^i g^i_{uu}$$

For $u=u^*$, this reduces to

$$H_{uu}(u^*,c) = f_{uu} + \sum_{i=1}^{m} \mu^i g^i_{uu} + \mu_u^T g_u + g_u^T \mu_u + 2cg_u^T g_u$$

or

$$H_{uu}(u^*,c) = L_{uu}(u^*,\lambda^*) + \mu_u^T g_u + g_u^T \mu_u + 2cg_u^T g_u$$

Now let Q be the subspace of R^n spanned by the rows of $g_u(u^*)$, and let $Q^\perp$ be the orthogonal complement. Since the constraint qualifications are assumed to hold at u^*, Q has dimension m. If $y_1 \in Q$ and $y_2 \in Q^\perp$, we then have $y_1^T y_2 = 0$, $g_u y_2 = 0$ and $y_1 = g_u^T \alpha$, where $\alpha \in R^m$ is uniquely determined by y_1. Similarly, we can choose an arbitrary basis $e_1, \ldots, e_{n-m}$ in $Q^\perp$. Then any $y_2 \in Q^\perp$ may be written

$$y_2 = \sum_{i=1}^{n-m} \beta_i e_i \qquad \text{or} \qquad y_2 = G\beta$$

where $\beta \in R^{n-m}$ and G is an $n\times(n-m)$-dimensional matrix of rank n-m. Conversely, $y_2 = G\beta$ lies in $Q^{\perp}$ for any $\beta \in R^{n-m}$. Then we may write an arbitrary vector $y \in R^n$ in the form

$$y = g_u^T\alpha + G\beta$$

Now consider $y^T H_{uu}(u^*,c)y$.

$$\begin{aligned} y^T H_{uu}(u^*,c)y &= (g_u^T\alpha+G\beta)^T H_{uu}(u^*,c)(g_u^T\alpha+G\beta) = \\ &= \alpha^T\Big\{2cg_u g_u^T g_u g_u^T + g_u L_{uu} g_u^T + \\ &\quad + g_u \mu_u^T g_u g_u^T + g_u g_u^T \mu_u g_u^T\Big\}\alpha + \\ &\quad + \alpha^T\Big\{g_u L_{uu} G + g_u g_u^T \mu_u G\Big\}\beta + \\ &\quad + \beta^T\Big\{G^T L_{uu} g_u^T + G^T \mu_u^T g_u g_u^T\Big\}\alpha + \\ &\quad + \beta^T\Big\{G^T L_{uu} G\Big\}\beta \end{aligned}$$

where all quantities are evaluated at $u=u^*$.

To get a better survey, we introduce

$$A(c) = 2cg_u g_u^T g_u g_u^T + g_u L_{uu} g_u^T + g_u \mu_u^T g_u g_u^T + g_u g_u^T \mu_u g_u^T$$

$$B = g_u L_{uu} G + g_u g_u^T \mu_u G$$

$$D = G^T L_{uu} G$$

Then

$$y^T H_{uu}(u^*,c)y = \begin{bmatrix}\alpha^T, \beta^T\end{bmatrix} \begin{bmatrix} A(c) & B \\ B^T & D \end{bmatrix} \begin{bmatrix}\alpha \\ \beta\end{bmatrix}$$

It now remains to prove the existence of a parameter c_0, such that

$$\begin{bmatrix} A(c) & B \\ B^T & D \end{bmatrix} > 0$$

for $c>c_0$.

This will be done in three steps. First A(c) is considered, and it is shown that for every real $k>0$, there exists a $c_0(k)$, such that $A(c)>kI_m$ for $c>c_0(k)$. Then we will prove that $D>0$, and finally it will be shown that

$$\begin{bmatrix} kI_m & B \\ B^T & D \end{bmatrix} > 0$$

for k large enough.

Consider

$$A(c) - kI_m = 2c(g_u g_u^T)(g_u g_u^T) + g_u L_{uu} g_u^T +$$

$$+ g_u \mu_u^T g_u g_u^T + g_u g_u^T \mu_u g_u^T - kI_m$$

Since the constraint qualifications hold at u^*, $g_u g_u^T$ is nonsingular, and $(g_u g_u^T)(g_u g_u^T)$ is positive definite symmetric. Then there exists a nonsingular transformation S(k) such that [7]

$$2(g_u g_u^T)(g_u g_u^T) = S^T(k)S(k)$$

and

$$g_u L_{uu} g_u^T + g_u \mu_u^T g_u g_u^T + g_u g_u^T \mu_u g_u^T - kI_m =$$

$$= S^T(k) \begin{pmatrix} a_1(k) & & 0 \\ & \ddots & \\ 0 & & a_m(k) \end{pmatrix} S(k)$$

This yields

$$A(c) - kI_m = S^T(k) \begin{pmatrix} c+a_1(k) & & 0 \\ & \ddots & \\ 0 & & c+a_m(k) \end{pmatrix} S(k)$$

and thus $A(c) - kI_m > 0$ for

$c > -\min_i a_i(k)$.

Next consider the matrix D. For every $y_2 \in Q^\perp$, $y_2 \neq 0$, we have

$$y_2^T L_{uu}(u^*,\lambda^*) y_2 > 0$$

according to Lemma 3. But any y_2 in $Q^\perp$ may be written $y_2 = G\beta$, and any vector $G\beta$ lies in $Q^\perp$. Then

$$\beta^T G^T L_{uu}(u^*,\lambda^*) G\beta > 0$$

for $\beta \neq 0$, which proves that $D = G^T L_{uu}(u^*,\lambda^*)G$ is positive definite.

Finally we will consider the matrix

$$\begin{bmatrix} kI_m & B \\ B^T & D \end{bmatrix}$$

Introduce the nonsingular transformation

$$L(k) = \begin{bmatrix} I_m & -\frac{1}{k} B \\ 0 & I_{n-m} \end{bmatrix}$$

Then

$$L^T(k) \begin{bmatrix} kI_m & B \\ B^T & D \end{bmatrix} L(k) = \begin{bmatrix} kI_m & 0 \\ 0 & \frac{1}{k}(kD-B^TB) \end{bmatrix}$$

and thus it is sufficient to prove that $kD - B^TB > 0$ for k large enough. But D is positive definite, and then there exists a nonsingular transformation T, such that

$$D = T^TT$$

and

$$B^TB = T^T \begin{bmatrix} b_1 & & 0 \\ & \ddots & \\ 0 & & b_m \end{bmatrix} T$$

Thus we have $kD - B^TB > 0$ for

$$k > \max_i b_i$$

This completes the proof of the existence of a finite c_0, such that $H_{uu}(u^*,c) > 0$ for $c>c_0$.

The theorem evidently breaks down if the problem is singular, i.e. D is only nonnegative definite. To be able to extend the multiplier function concept to this case, it is natural to require that H(u,c) should have the properties

$$H_u(u^*,c) = 0$$

$$H_{uu}(u^*,c) \geq 0$$

independent of the character of the optimal solution. We will now prove, that this is attained by including the condition iii) in the definition of the multiplier functions.

Theorem 3

Let u^* be a local minimum of f(u) subject to the constraints g(u) = 0. Then there exists a c_0, such that $H_u(u^*,c) = 0$ and $H_{uu}(u^*,c) \geq 0$ for $c>c_0$.

Proof: It is necessary and sufficient to prove that

$$kD - B^T B \geq 0$$

for k large enough. The theorem will then follow from the proof of Theorem 2.

Since D may be singular, a necessary condition obviously is

$$B\beta = 0$$

for every $\beta \in R^{n-m}$, such that

$$\beta^T D\beta = 0$$

But from the definition of B, D and β follows that this is equivalent to

$$(g_u L_{uu} + g_u g_u^T \mu_u)y = 0$$

for every $y \in R^n$, such that

$$g_u y = 0$$

and

$$y^T L_{uu} y = 0$$

Thus condition iii) is a necessary condition for $H_{uu}(u^*,c) \geq 0$. To prove that iii) is a sufficient condition (together with i) and ii)), and to get a measure of k, assume that rank $D = r$, $0 < r < (n-m)$. Then D may be written

$$D = D_1^T D_1$$

where D_1 is an $r\times(n-m)$ matrix of rank r. Let P be the subspace of R^{n-m} spanned by the rows of D_1, and let $P^\perp$ be the orthogonal complement. Then every $\beta \in R^{n-m}$ may be uniquely decomposed into

$$\beta = D_1^T\gamma + \beta_2$$

where $D_1^T\gamma \in P$ and $\beta_2 \in P^\perp$. Since $D_1\beta_2 = 0$, $\forall \beta_2 \in P^\perp$, it follows that $\beta_2^T D_1^T D_1 \beta_2 = \beta_2^T D\beta_2 = 0$, and thus $B\beta_2 = 0$

according to condition iii). Then

$$\beta^T(kD - B^TB)\beta = (D_1^T\gamma + \beta_2)^T(kD_1^TD_1 - B^TB)(D_1^T\gamma + \beta_2) =$$

$$= \gamma^T\left[k(D_1D_1^T)(D_1D_1^T) - D_1B^TBD_1^T\right]\gamma$$

But $(D_1D_1^T)(D_1D_1^T)$ is positive definite symmetric and then there exists a nonsingular transformation V such that

$$(D_1D_1^T)(D_1D_1^T) = V^TV$$

and

$$D_1B^TBD_1^T = V^T\begin{pmatrix} s_1 & & 0 \\ & \ddots & \\ 0 & & s_r \end{pmatrix}V$$

Thus

$$\beta^T(kD - B^TB)\beta \geq 0, \quad \beta \in R^{n-m}$$

for

$$k \geq \max_i s_i.$$

We have then proved the existence of a finite c_0, such that $H_{uu}(u^*,c) \geq 0$ for $c>c_0$.

4. EXAMPLES.

To illustrate the multiplier function concept, some particular choices of $\mu(u)$ are investigated in this section. We will also try to make clear by examples, how different choices of $\mu(u)$ may result in different properties of the generalized Lagrangian. The possibility to generate different generalized Lagrangians is of great importance for the numerical solution of the optimization problem.

Example 1

Assume that the optimal multipliers λ^* are à priori known. A simple choice of the multiplier function might then be

$$\mu(u) = \lambda^* = \text{const.}$$

This special case has been considered by Hestenes [3]. It may seem strange to assume the optimal multipliers to be à priori known, when the optimal solution is not known. The reason for this will become clear in the next section, where computational methods based on successive estimations of λ^* are considered. It is then important to establish properties of

$$H_i(u,c) = f(u) + \lambda_i^T g(u) + cg^T(u)g(u)$$

as λ_i tends to the optimal multipliers λ^*.

For nonsingular problems, $\mu(u) = \lambda^*$ obviously is an admissible multiplier function since it trivially satisfies conditions i) and ii) of the multiplier function definition. In the singular case, however, it depends on the particular problem whether $\mu(u) = \lambda^*$

satisfies condition iii) or not. This condition becomes particularly simple for this multiplier function. Consider

$$(g_u L_{uu} + g_u g_u^T \mu_u) y_2 = g_u L_{uu} y_2 = 0$$

Thus $L_{uu} y_2 \in Q^{\perp}$, where $Q^{\perp}$ is the orthogonal complement of the subspace spanned by the rows of g_u. But in the singular case, there exists $y_2 \in Q^{\perp}$, $y_2 \neq 0$, such that

$$y_2^T L_{uu} y_2 = 0$$

and thus $L_{uu} y_2 \in Q$. Since $Q \cap Q^{\perp} = \{0\}$, the condition iii) then reduces to $L_{uu} y_2 = 0$.

Consider the following simple singular problem. Minimize

$$f(u) = (u_1 - u_2)^2$$

subject to the constraint

$$g(u) = u_1 - u_2 = 0 \qquad \text{(Problem 1)}$$

Choosing $y_2^T = (\alpha, \alpha)$, $g_u y_2 = 0$ and $y_2^T L_{uu} y_2 = 0$ for any value of α. But $L_{uu} y_2 = 0$ and thus $\mu(u) = \lambda^* = 0$ is an admissible multiplier function. In this case the generalized Lagrangian is $H(u,c) = (1+c)(u_1-u_2)^2$.

For the following problem $\mu(u) = \lambda^*$ is not a multiplier function. Minimize

$$f(u) = u_1^2 - u_2^2$$

subject to

$$g(u) = u_1 + u_2 = 0 \qquad \text{(Problem 2)}$$

Choosing $y_2^T = (\alpha,-\alpha)$, $g_u y_2 = 0$, $y_2^T L_{uu} y_2 = 0$ but $L_{uu} y_2 \neq 0$, $\alpha \neq 0$. The generalized Lagrangian becomes $H(u,c) = u_1^2 - u_2^2 + \lambda^*(u_1+u_2) + c(u_1+u_2)^2$, or

$$H(u,c) = \frac{1}{2}(u-u^*)^T \begin{pmatrix} 2c+2 & 2c \\ 2c & 2c-2 \end{pmatrix} (u-u^*)$$

where u^* is the optimal solution corresponding to the particular choice of λ^* (λ^* turns out to be arbitrary). It is easily verified, that for this problem, the optimal solution u^* cannot be made a minimum of $H(u,c)$ by choosing c large enough. To prove this, choose $\bar{u}^T = \left(u_1^* - 2c\alpha/(2c+2),\ u_2^* + \alpha\right)$. Then

$$H(\bar{u},c) - H(u^*,c) = -4\alpha^2$$

for any finite c, and thus $H(u^*,c) > H(\bar{u},c)$ if $\alpha \neq 0$.

Example 2

To avoid the trouble associated with singular problems, one obviously should look for a multiplier function that satisfies the conditions i) - iii) for any character of the problem. One possibility to achieve this is to choose

$$\mu(u) = -\left(g_u(u) g_u^T(u)\right)^{-1} g_u(u) f_u^T(u)$$

This multiplier function has been investigated by Mårtensson [4] and Fletcher [5]. Assuming f(u) and

$g(u)$ three times differentiable in a neighbourhood of u^*, it can be shown [4], that $\mu(u)$ exists and is twice differentiable in a neighbourhood of u^*, that $\mu(u^*) = \lambda^*$, and that $g_u(u^*)L_{uu}(u^*,\lambda^*) + g_u(u^*)g_u^T(u^*) \cdot \mu_u(u^*) = 0$. Thus $\mu(u)$ is an admissible multiplier function for both singular and nonsingular problems.

With this choice of multiplier function, we get the same generalized Lagrangian for Problem 1 as in the previous example, namely $H(u,c) = (1+c)(u_1-u_2)^2$. However, for Problem 2, the generalized Lagrangian now becomes $H(u,c) = c(u_1+u_2)^2$, and this possesses all the desired properties.

We will illustrate the multiplier function concept with one more simple problem. This also illustrates the possibility of handling inequality constraints by means of slack variables. Minimize

$$f(u) = -\frac{16}{3} u_1^3 - 2u_1^2 + 2u_1$$

subject to the constraint

$$u_1 - 1 \leq 0 \qquad \text{(Problem 3)}$$

The problem has two local isolated minima, one at the constraint $u_1=1$, and one at $u_1=-0.5$. The inequality constraint may be transformed into an equality constraint by adding a slack variable u_2 in such a way that the constraint qualifications of Lemma 1 are satisfied, e.g.

$$g(u) = u_1 - 1 + u_2^2 = 0$$

In Fig. 1, contour levels of $H(u,c)$ are drawn for $c=0$, 1.0 and 5.0. Since H is symmetric with respect to u_2, the contour levels are drawn only for $u_2 \geq 0$. From the figure it is clear that any minimization method should be able to reach one of the minima if we choose c large enough, and if the initial guess is not too far from the curve representing the equality constraint $g(u) = 0$. For further examples of the slack variable technique, we refer to [4].

Example 3

In this example we will indicate some obvious generalizations of the preceding example.

One drawback of the multiplier function

$$\mu(u) = - (g_u g_u^T)^{-1} g_u f_u^T$$

is that $(g_u g_u^T)$ may be singular for some u outside the equality constraint. A possible way to overcome this, is to choose

$$\mu(u) = - (g_u g_u^T + g^T g \; I_m)^{-1} g_u f_u^T$$

It is easily verified that this is an admissible multiplier function for both singular and nonsingular problems.

It is also clear from Fig. 1, that one may get into trouble if the initial guess of the optimal solution is too far away from the curve representing the constraint. To get the right slope of H(u,c), but preserving its smooth character around the optimal solution, one could select

$$\mu(u) = - (g_u g_u^T)^{-1} g_u f_u^T + (g^T g)^n g$$

The multiplier functions considered in this section have been explicite functions with similar basic structure. An interesting problem is then, whether there exist multiplier functions with different structures or not. It may also be of great interest to try to define the multiplier function implicitely. These problems have not yet been investigated.

5. ALGORITHMS AND COMPUTATIONAL ASPECTS.

A number of different algorithms can be designed for the minimization of the generalized Lagrangian H(u,c). Roughly they can be separated into two major classes, direct minimization of H(u,c) with ordinary function minimization methods, and iterative estimation of the multiplier function $\mu(u)$. Although the latter methods require iteration in a larger space, they can be made very efficient by using the function properties of the multiplier $\mu(u)$.

Direct Minimization Methods.

A straightforward way to minimize H(u,c) is to use a minimization method where only function value evaluations are required, e.g. the methods of Powell [8] and Stewart [9]. Stewart's method, which is a modification of Davidon's method [10], is generally considered to be somewhat more efficient since difference approximations of the derivatives can be used. However, as was illustrated in Section 4, the multiplier functions must be chosen carefully since we do not have any à priori estimate of the parameter c.

This problem can to some extent be avoided if it is possible to evaluate μ_u. Then the derivative

$$H_u = f_u + \mu^T g_u + g^T \mu_u + 2cg^T g_u$$

of H(u,c) can be computed, and a more efficient minimization method can be used, e.g. the method of Fletcher and Powell [11]. But it will also be possible to get an à priori estimate of c, and thereby make the minimization of H(u,c) less sensitive to the particular choice of $\mu(u)$.

Consider the quantity $g^T(u)g(u)$, which equals zero if and only if the constraints are satisfied. If it is required that H(u,c) has the property

$$\left[\frac{d}{du}(g^Tg)\right]H_u^T > 0$$

then the magnitude of g^Tg can be decreased by moving in the direction opposite to H_u, that is, in the steepest descent direction. But

$$\left[\frac{d}{du}(g^Tg)\right]H_u^T = 2g^Tg_u(f_u + \mu^Tg_u + g^T\mu_u + 2cg^Tg_u)^T$$

and then this condition is satisfied if

$$c > -\frac{g^Tg_u(f_u^T + g_u^T\mu + \mu_u^Tg)}{2g^Tg_ug_u^Tg}$$

for $g(u) \neq 0$. Further properties of this measure are discussed in [4].

Multiplier Estimation Methods.

An obvious disadvantage of direct minimization methods is the time-consuming function and gradient evaluations that have to be carried out for every step. It then seems reasonable that methods based on iterative estimation of the optimal multipliers could be made more efficient than the direct minimization methods.

In this section, different estimation algorithms are derived, and they will be classified according to their convergence properties for quadratic functions with linear constraints.

Consider the following simple iteration scheme:
Make an initial guess of λ^*, say μ_k (subscripts will be used to denote the iteration step). Then minimize $F(u,\mu_k) = f(u) + \mu_k^T g(u) + cg^T(u)g(u)$ with an efficient minimization method. Assume that the minimum occurs for $u = u_{k+1}$. If $g(u_{k+1}) \leq \delta$, where δ is a small quantity, then u_{k+1} is the optimal solution. Otherwise compute a new estimate $\mu_{k+1} = \mu(u_{k+1})$ and repeat the procedure.

Notice that the algorithm does not depend on any particular choice of the multiplier function $\mu(u)$. It is then natural to examine if $\mu(u)$ can be selected so that the algorithm is further simplified.

Assume that u_{k+1} minimizes $F(u,\mu_k)$. Then

$$f_u(u_{k+1}) + \mu_k^T g_u(u_{k+1}) + 2cg^T(u_{k+1})g_u(u_{k+1}) = 0$$

and post-multiplying by $g_u^T(u_{k+1})[g_u(u_{k+1})g_u^T(u_{k+1})]^{-1}$, we get

$$f_u(u_{k+1})g_u^T(u_{k+1})\left[g_u(u_{k+1})g_u^T(u_{k+1})\right]^{-1} + \mu_k^T + 2cg^T(u_{k+1}) = 0$$

From this we conclude that $\mu(u) = -(g_u g_u^T)^{-1} g_u f_u^T$ is a suitable choice of the multiplier function, since the new estimate μ_{k+1} then satisfies

$$-\mu_{k+1}^T + \mu_k^T + 2cg^T(u_{k+1}) = 0$$

or

$$\mu_{k+1} = \mu_k + 2cg(u_{k+1})$$

This will drastically reduce the computations involved. It is also interesting to notice, that this recursive relation, which also has been suggested by Hestenes [3], can be considered as a special case of a more general estimation algorithm.

The algorithm can then be summarized as follows:

First order algorithm:

a) Set $\mu_k = 0$

b) Minimize $F(u,\mu_k) = f(u) + \mu_k^T g(u) + cg^T(u)g(u)$ with an ordinary function minimization algorithm, e.g. Fletcher-Powell. Notice that the evaluations of the function value and of the gradient are very simple. Assume that the minimum occurs for $u = u_{k+1}$.

c) If $\| g(u_{k+1}) \| \leq \delta$, where δ is a small quantity, then $u^* = u_{k+1}$.

d) If $\| g(u_{k+1}) \| > \delta$, set $\mu_{k+1} = \mu_k + 2cg(u_{k+1})$ and return to b).

It is possible to establish convergence properties of the algorithm for quadratic functions with linear constraints.

Theorem 4

Let f(u) be quadratic, and assume that the constraint g(u) is linear. If $\mu(u) = \lambda^*$ is an admissible multiplier function for the problem, the algorithm converges to the optimal solution for $c > \max(0,2c_0)$.

Proof: Consider the situation at stage k. Since u_{k+1} minimizes $F(u,\mu_k)$, we have

$$f_u(u_{k+1}) + \mu_k^T g_u(u_{k+1}) + 2cg^T(u_{k+1})g_u(u_{k+1}) = 0$$

or

$$f_u(u_{k+1}) + \mu_{k+1}^T g_u(u_{k+1}) = 0$$

At stage k+1, u_{k+2} minimizes $F(u,\mu_{k+1})$, and

$$f_u(u_{k+2}) + \mu_{k+1}^T g_u(u_{k+2}) + 2cg^T(u_{k+2})g_u(u_{k+2}) = 0$$

Combining these conditions, and expanding f(u) and g(u) yields

$$2cg^T g_u = (u_{k+1} - u_{k+2})^T f_{uu} - 2cu_{k+2}^T g_u^T g_u$$

where all quantities are evaluated at u=0. Then consider the identity

$$c\left[g^T(u_{k+2})g(u_{k+2}) - g^T(u_{k+1})g(u_{k+1})\right] =$$

$$= cu_{k+2}^T g_u^T g_u u_{k+2} - cu_{k+1}^T g_u^T g_u u_{k+1} + 2cg^T g_u(u_{k+2} - u_{k+1})$$

Insert the expression for $2cg^T g_u$ and rearrange the terms to get

$$c\left[g^T(u_{k+2})g(u_{k+2}) - g^T(u_{k+1})g(u_{k+1})\right] =$$

$$= -(u_{k+2} - u_{k+1})^T(f_{uu} + cg_u^T g_u)(u_{k+2} - u_{k+1})$$

Since $\mu(u) = \lambda^*$ is assumed to be an admissible multiplier function,

$$f_{uu} + cg_u^T g_u \geq 0$$

for $c>2c_0$ according to Theorem 3, and we then have to investigate two different cases separately.

Assume that $f_{uu} + cg_u^T g_u > 0$ for $c>2c_0$. Then

$$g^T(u_{k+2})g(u_{k+2}) < g^T(u_{k+1})g(u_{k+1})$$

for $c > \max(0,2c_0)$ provided that $u_{k+2} \neq u_{k+1}$. Since $|| g(\cdot) || \geq 0$, $g^T(u_i)g(u_i)$ will converge either to zero or to a finite $G>0$. In the latter case we get $u_{i+2} = u_{i+1}$ and $\mu_{i+2} = \mu_{i+1}$. But $\mu_{i+2} = \mu_{i+1} + 2cg(u_{i+2})$, which proves that $u_{i+2} = u_{i+1}$ if and only if $g(u_{i+2}) = g(u_{i+1}) = 0$. Thus the algorithm converges for non-singular problems.

Then consider the singular case, that is, there exists $y_2 \neq 0$, such that $y_2^T(f_{uu} + cg_u^T g_u)y_2 = 0$, $c > \max(0,2c_0)$. Then, according to the multiplier function definition and to Theorem 3, $g_u y_2 = 0$ and $L_{uu}y_2 = f_{uu}y_2 = 0$. This implies that

$$2cg^T g_u = (u_{k+1} - u_{k+2})^T f_{uu} - 2cu_{k+2}^T g_u^T g_u$$

reduces to

$$2cg^T(u_{k+2})g_u = 0$$

and then $g(u_{k+2}) = 0$, $c>0$, since g_u is assumed to satisfy the constraint qualifications, i.e. to have full rank. This completes the convergence proof of algorithm.

It is instructive to verify the convergence for the following simple example. Minimize

$$f(u) = u_1^2 - u_2^2$$

subject to

$$u_1 - 2u_2 - 2 = 0$$

For this problem $c_0 = \frac{1}{3}$, and for $c > \frac{2}{3}$ the algorithm converges to the optimal solution $u_1 = -\frac{2}{3}$, $u_2 = -\frac{4}{3}$. For $c < \frac{2}{3}$ the algorithm diverges, while for $c = \frac{2}{3}$ the quantity $g^T(u_i)g(u_i)$ is constant.

The convergence rate depends on the choice of c. Introduce $\varepsilon_k = || g(u_k) ||$ and choose c=1. The following residuals are then obtained:

$$\varepsilon_{k+1} = \frac{1}{2}\varepsilon_k \qquad \varepsilon_1 = 1$$

Increasing c to c=5, convergence is improved considerably, and the residuals are

$$\varepsilon_{k+1} = \frac{1}{14}\varepsilon_k \qquad \varepsilon_1 = \frac{1}{7}$$

So far, the multiplier function concept has been used only for estimation of the optimal multipliers. The properties of $\mu(u)$ will now be exploited to develop second order algorithms, that is, algorithms with one-step convergence for linear-quadratic problems. The following theorem will be required.

Theorem 5

Let u^* minimize $f(u)$ subject to the constraints $g(u) = 0$, and assume that the sufficient conditions of Lemma 3 are satisfied. Define the projection $P(u)$ as

$$P(u) = I_n - g_u^T(u)\left[g_u(u)g_u^T(u)\right]^{-1} g_u(u)$$

Then

$$P(u^*)L_{uu}(u^*,\lambda^*) + 2cg_u^T(u^*)g_u(u^*)$$

is nonsingular for $c \neq 0$.

Proof: The theorem is proved by contradiction. Assume that $PL_{uu} + 2cg_u^Tg_u$ is singular, and that there exists $z \neq 0$, such that $z^T(PL_{uu} + 2cg_u^Tg_u) = 0$. Decompose z into $z = g_u^T\alpha + z_2$, where $g_u^T\alpha \in Q$, the space spanned by the rows of g_u, and $z_2 \in Q^\perp$. Then $z^T(PL_{uu} + 2cg_u^Tg_u) = 0$ is equivalent to

$$2c\alpha^T(g_ug_u^T)g_u + z_2^TL_{uu} = 0$$

since $g_uP = 0$ and $z_2^TP = z_2^T$. Now assume that there exists $z_2 \neq 0$, such that $2c\alpha^T(g_ug_u^T)g_u + z_2^TL_{uu} = 0$. Postmultiplying by z_2 then yields

$$z_2^TL_{uu}z_2 = 0$$

which contradicts the assumption that $z_2^TL_{uu}z_2 > 0$ for $z_2 \neq 0$ (Lemma 3). If $z_2 = 0$, $\alpha \neq 0$, then $\alpha^T(g_ug_u^T)g_u = 0$ for $c \neq 0$, which contradicts the constraint qualification, i.e. the linear independence of the rows of g_u. Thus, for $c \neq 0$, there is no nonzero solution, and $P(u^*)L_{uu}(u^*,\lambda^*) + 2cg_u^T(u^*)g_u(u^*)$ is nonsingular.

<u>Corollary</u>

If $f(u)$ is quadratic and the constraints $g(u)$ are linear, then

$$Pf_{uu} + 2cg_u^T g_u$$

is nonsingular for $c \neq 0$.

Proof: $Pf_{uu} + 2cg_u^T g_u$ is independent of u and is nonsingular for $u=u^*$.

Using these results, we will now design a second order estimation method. Assume that an estimate μ_k of the optimal multipliers $\lambda^* = \mu_k + \delta\mu_k$ is available. Let $u^* = u_{k+1} + \delta u_{k+1}$, where u_{k+1} minimizes $F(u,\mu_k)$, be the optimal solution. Approximate $F_u(u^*,\lambda^*)$ with a first order series expansion about u_{k+1}, μ_k. Then

$$F_u(u^*,\lambda^*) = F_u(u_{k+1},\mu_k) + F_{uu}(u_{k+1},\mu_k)\delta u_{k+1} +$$

$$+ F_{u\mu}(u_{k+1},\mu_k)\delta\mu_k = 0$$

Since $F_u(u_{k+1},\mu_k) = 0$, this reduces to

$$F_{uu}(u_{k+1},\mu_k)\delta u_{k+1} + F_{u\mu}(u_{k+1},\mu_k)\delta\mu_k = 0$$

In contrast to the first order algorithm, the quantity $\delta\mu_k$ is now unknown. But $\mu(u)$ is a function of u, and so we make the following approximation of $\delta\mu_k$.

$$\delta\mu_k = \mu(u_{k+1}) - \mu(u_k) + \mu_u(u_{k+1})\delta u_{k+1}$$

Now choose the particular multiplier function $\mu(u) = -(g_u g_u^T)^{-1} g_u f_u^T$. Then

$$\delta\mu_k = 2cg(u_{k+1}) + \mu_u(u_{k+1})\delta u_{k+1}$$

Inserting this into the series expansion, we get

$$F_{uu}\delta u_{k+1} + F_{u\mu}\delta\mu_k = F_{uu}\delta u_{k+1} + 2cF_{u\mu}g + F_{u\mu}\mu_u\delta u_{k+1} = 0$$

where all quantities are evaluated at u_{k+1}, μ_k. Noticing that $F_{u\mu} = g_u^T$, this is equivalent to

$$\left[f_{uu} + \sum_{i=1}^{m} \mu_k^i g_{uu}^i + 2cg_u^T g_u + 2c \sum_{i=1}^{m} g^i g_{uu}^i + g_u^T \mu_u\right]\delta u_{k+1} +$$

$$+ 2cg_u^T g = 0$$

or

$$\left[f_{uu} + \sum_{i=1}^{m} \mu_{k+1}^i g_{uu}^i + 2cg_u^T g_u + g_u^T \mu_u\right]\delta u_{k+1} + 2cg_u^T g = 0$$

To evaluate $\mu_u(u_{k+1})$, we have to differentiate the multiplier function $\mu(u) = -(g_u g_u^T)^{-1} g_u f_u^T$. It is then easily verified that

$$\mu_u(u_{k+1}) = -(g_u g_u^T)^{-1} g_u\left[f_{uu} + \sum_{i=1}^{m} \mu_{k+1}^i g_{uu}^i\right]$$

and thus

$$\left[P\left[f_{uu} + \sum_{i=1}^{m} \mu_{k+1}^i g_{uu}^i\right] + 2cg_u^T g_u\right]\delta u_{k+1} + 2cg_u^T g = 0$$

where P is the projection matrix

$$P = I_n - g_u^T(g_u g_u^T)^{-1} g_u$$

In Theorem 5 it was shown that $P(u^*)L_{uu}(u^*,\lambda^*) + 2cg_u^T(u^*)g_u(u^*)$ is nonsingular for $c \neq 0$, so that for u_{k+1} sufficiently close to u^*, we get

$$\delta u_{k+1} = - \left(P(u_{k+1})L_{uu}(u_{k+1},\mu_{k+1}) + \right.$$

$$\left. + 2cg_u^T(u_{k+1})g_u(u_{k+1})\right)^{-1} 2cg_u^T(u_{k+1})g(u_{k+1})$$

For the linear-quadratic problem, this will yield the optimal solution $u^* = u_{k+1} + \delta u_{k+1}$ in one step. Also notice, that in case g_u is nonsingular, $\delta u_{k+1} = - g_u^{-1}(u_{k+1})g(u_{k+1})$, that is, u^* is determined by the condition $g(u^*) = 0$.

Summarizing, we get the following algorithm:

Second order algorithm I:

a) Select $\mu_k = 0$.

b) Minimize $F(u,\mu_k)$ with an ordinary function minimization algorithm. Assume that the minimum occurs for $u = u_{k+1}$.

c) If $\| g(u_{k+1}) \| < \delta$, where δ is a small quantity, then $u^* = u_{k+1}$.

d) Compute

$$\mu_{k+1} = \mu_k + 2cg(u_{k+1})$$

$$G = P(u_{k+1})L_{uu}(u_{k+1},\mu_{k+1}) + 2cg_u^T(u_{k+1})g_u(u_{k+1})$$

and

$$\delta u_{k+1} = - 2cG^{-1}g_u^T(u_{k+1})g(u_{k+1})$$

If G is singular, return to b) and minimize $F(u,\mu_{k+1})$.

e) Estimate $\mu_{k+2} = \mu(u_{k+1} + \delta u_{k+1})$ and return to b).

Notice that this algorithm depends heavily on the particular choice of $\mu(u)$. To allow for arbitrary multiplier functions, one possibility is to simply approximate $\mu(u)$ by the series expansion

$$\mu(u) = \mu(u_k) + \mu_u(u_k)(u-u_k)$$

We then have

Second order algorithm II:

a) Set $\mu(u_k) = 0$ and $\mu_u(u_k) = 0$.

b) Minimize $f(u) + [\mu(u_k) + \mu_u(u_k)(u-u_k)]^T g(u) + $ $+ 2cg^T(u)g(u)$ with an ordinary minimization algorithm. Assume that the minimum occurs for $u = u_{k+1}$.

c) If $|| g(u_{k+1}) || < \delta$, then $u^* = u_{k+1}$.

d) Compute $\mu(u_{k+1})$ and $\mu_u(u_{k+1})$ and return to b).

The function and gradient evaluations at stage b) are still very simple, since $\mu(u_k)$ and $\mu_u(u_k)$ are evaluated only at the minimizing point u_k. The convergence properties of the algorithm depend on the choice of $\mu(u)$. In particular, if $\mu(u) = -(g_u g_u^T)^{-1} g_u f_u^T$ the algorithm has one-step convergence for linear-quadratic problems for $c>c_0$. In this case the approximation of $\mu(u)$ is exact.

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7. REFERENCES.

[1] A.V. Fiacco and G.P. McCormick: "Nonlinear Programming: Sequential Unconstrained Minimization Techniques", J. Wiley and Sons, New York, 1968.

[2] M.J.D. Powell: "A Method for Nonlinear Constraints in Minimization Problems", in R. Fletcher, ed.: "Optimization", Academic Press, London, 1969.

[3] M.R. Hestenes: "Multiplier and Gradient Methods", J. Opt. Theory Appl., 4, No. 5, 1969, 303 - 320.

[4] K. Mårtensson: "Methods for Constrained Function Minimization", Research Report 7101, March, 1971, Lund Institute of Technology, Division of Automatic Control.

[5] R. Fletcher: "Methods for Nonlinear Programming", in J. Abadie, ed.: "Integer and Nonlinear Programming", North-Holland Publishing Company, 1970.

[6] O.L. Mangasarian: "Nonlinear Programming", McGraw-Hill, 1968.

[7] F.R. Gantmacher: "The Theory of Matrices", Chelsea Publishing Company, New York, 1960.

[8] M.J.D. Powell: "An Efficient Method for Finding the Minimum of a Function of Several Variables without Calculating Derivatives", Computer Journal, 7, No. 2, 1964, 155 - 162.

[9] G.W. Stewart III: "A Modification of Davidon's Minimization Method to Accept Difference Approximations to Derivatives", J. Ass. Comput. Mach., 14, No. 1, 1967, 72 - 83.

[10] W.C. Davidon: "Variable Metric Method for Minimization", AEC Research and Development Report ANL 5990, 1959.

[11] R. Fletcher and M.J.D. Powell: "A Rapidly Convergent Descent Method for Minimization", Computer Journal, 6, No. 2, 1963, 163 - 168.