Methods for Constrained Function Minimization

Mårtensson, Krister

1971

LUND UNIVERSITY

PO Box 117
221 00 Lund
+46 46-222 00 00

METHODS FOR CONSTRAINED FUNCTION MINIMIZATION

K. MÅRTENSSON

REPORT 7101 MARCH 1971
LUND INSTITUTE OF TECHNOLOGY
DIVISION OF AUTOMATIC CONTROL

METHODS FOR CONSTRAINED FUNCTION MINIMIZATION†

K. Mårtensson

ABSTRACT.

A method for the minimization of a function $f(u)$ subject to the nonlinear constraints $g(u) = 0$, $h(u) \leq 0$, is presented. It is shown that the problem may be converted into an unconstrained well-conditioned minimization problem, where ordinary minimization methods can be applied.

---

† This work was supported by the Swedish Board for Technical Development (Contract 70-337/U270).

TABLE OF CONTENTS

1. INTRODUCTION.

In this paper a method for constrained function optimization is presented. The problem is to determine the n-dimensional vector u^*, which minimizes the function f(u) subject to the constraints g(u) = 0 and h(u) $\leq$ 0. g(u) and h(u) are the m-dimensional and p-dimensional vectors

$$g(u) = \begin{bmatrix} g^1(u) \\ \\ g^m(u) \end{bmatrix} \qquad h(u) = \begin{bmatrix} h^1(u) \\ \\ h^p(u) \end{bmatrix}$$

Many different methods for the solution of equality constrained problems (g(u) = 0) have been published. Generally these are based on one of two main ideas. The first is the Lagrange multiplier technique, where the constraints are adjoined by means of multipliers η, to form the Lagrangian

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

The problem then is to find a saddle-point in the u-η space, and thus the dimension of the problem is increased from n to n+m. The other basic approaches are penalty function methods. A function including the constraints in a proper manner is then added to the original function f(u), e.g.

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

Generally the optimal solution of $f(u) + cg^T(u)g(u)$ approaches the optimal solution of f(u) subject to the constraints as c tends to infinity. However, this method is less attractive from a numerical point of view, since it will create functions which are badly suited for numerical optimization. Different ways around this difficulty has been suggested e.g. by Fiacco and McCormick [1] and by Powell [3]. The main idea in these papers is to change the penalty function in an iterative way to make the optimum of the penalty function agree with the optimal solution. However, this often includes a set of new parameters to be iterated on, and then again the dimension of the problem is increased.

The method presented in this paper is in a sense a combination of the two basic methods. An m-dimensional vector function

$$\mu(u) = \begin{bmatrix} \mu^1(u) \\ \\ \mu^m(u) \end{bmatrix}$$

is defined as

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

where

$$g_u = \begin{bmatrix} g^1_{u_1} & \cdots & g^1_{u_n} \\ \vdots & & \vdots \\ g^m_{u_1} & \cdots & g^m_{u_n} \end{bmatrix}.$$

Conditions that guarantee nonsingularity of $(g_u g_u^T)$ are assumed to hold in a neighbourhood of u^*.

In section 3 properties of $\mu(u)$ are established, and it is shown that for the optimal solution $\mu(u)$ equals the optimal Lagrange multipliers. A generalized Lagrangian is then defined as

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

Using well-known results, which are given as lemmas in section 2, it is shown that H(u) has an extremum at $u = u^*$. It is also shown that there exists a finite parameter c_0, such that for $c > c_0$ $(c < c_0)$, H(u) has a local isolated minimum (maximum) at u^*, provided that the optimization problem has a local isolated minimum at u^*. Contrary to the penalty function method, there thus is a finite value of c, for which the unconstrained optimum of the generalized Lagrangian agrees with the solution of the optimization problem. Further, the dimension of the problem is independent of the number of constraints.

Inequality constraints are considered in section 4. These are handled by introducing slack variables so that the constraints are transformed into equalities. Results similar to those of section 3 are proved.

Two examples which illustrate the method are given in section 5, and numerical aspects are discussed. The major problem, namely the à priori choice of the parameter c is discussed, and a possible measure of c_0 is given. Some numerical experiences are also presented.

Since this paper was prepared, the same idea has been published by Fletcher [7]. However, it is focused upon methods using only function evaluations, while in this paper it is found that minimization methods using gradients seem to be necessary for an efficient minimization. It is also thought that this paper presents more efficient à priori estimates of the parameter c_0, both from theoretical and computational points of view.

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

In this section necessary and sufficient conditions for a local isolated minimum are stated. For proofs and a more detailed treatment we refer to [1].

Introduce the Lagrangian $L(u,\eta,\lambda)$ associated with the minimization problem stated in section 1.

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

where η^i are components of the m-dimensional vector η, and λ^j of the p-dimensional vector λ. These are generally called the Lagrange multipliers. We then have

<u>Lemma 1</u> (Existence theorem)

If

i) u^* satisfies the constraints $g(u^*) = 0$, $h(u^*) \leq 0$

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

iii) at u^* the set

$$Z = \left\{z;\ z^T g_u^i = 0,\ z^T h_u^j \leq 0,\ z^T f_u < 0\right\}$$

is empty

then there exists an m-dimensional vector $\eta = \{\eta^i\}$ and a p-dimensional vector $\lambda = \{\lambda^i\}$, such that

$$g^i(u^*) = 0 \qquad i = 1, \ldots, m$$

$$h^j(u^*) \leq 0 \qquad j = 1, \ldots, p$$

$$\lambda^j h^j(u^*) = 0 \qquad j = 1, \ldots, p$$

$$\lambda^j \geq 0 \qquad j = 1, \ldots, p$$

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

Different conditions which assure that the set Z is empty, and thus guarantee the existence of the Lagrange multipliers, can be stated [1], [2]. The most valuable from a computational point of view is the following.

Lemma 2 (Constraint qualification theorem)

A sufficient condition for the set Z to be empty, and thus for the existence of finite Lagrange multipliers η and λ, is that the gradients $\{g_u^i\}$ $\{h_u^j\}$ are linearly independent at u^*.

Notice, that this is a sufficient condition for the existence of η and λ. For some problems it may fail, and then it is still an open question, whether finite multipliers exist or not. In the following it is assumed that the sufficient condition of lemma 2 holds.

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

Lemma 3

If f, $\{g^i\}$ and $\{h^j\}$ are twice continuously differentiable at u^*, and if the constraints qualifications of lemma 2 hold at u^*, then a necessary condition for u^* to be a local minimum is the existence of vectors η and λ such that

$$g^i(u^*) = 0 \qquad i = 1, \ldots, m$$

$$h^j(u^*) \leq 0 \qquad j = 1, \ldots, p$$

$$\lambda^j h^j(u^*) = 0 \qquad j = 1, \ldots, p$$

$$\lambda^j \geq 0 \qquad j = 1, \ldots, p$$

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

Further, for every vector y such that $y^T h_u^j = 0$, $j \in B = \{j;\ h^j(u^*) = 0\}$, and $y^T g_u^i = 0$, $i = 1, \ldots, m$, it follows that

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

Sufficient second-order conditions for a local minimum is given by the following theorem.

Lemma 4

Sufficient conditions for u^* to be an isolated local minimum are that there exist vectors η and λ such that

$$g^i(u^*) = 0 \qquad i = 1, \ldots, m$$

$$h^j(u^*) \leq 0 \qquad j = 1, \ldots, p$$

$$\lambda^j h^j(u^*) = 0 \qquad j = 1, \ldots, p$$

$$\lambda^j \geq 0 \qquad j = 1, \ldots, p$$

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

Further, for every nonzero vector y such that $y^T h_u^j = 0$, $j \in D = \{j;\ h^j(u^*) = 0,\ \lambda^j > 0\}$, $y^T h_u^j \geq 0$, $j \in B - D = \{j;\ h^j(u^*) = 0,\ \lambda^j = 0\}$, $y^T g_u^i = 0$, $i = 1, \ldots, m$, it follows that

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

3. LAGRANGE MULTIPLIER FUNCTIONS. EQUALITY CONSTRAINTS.

The Lagrange multiplier technique for constrained minimization is very attractive from a theoretical point of view, but generally of limited value for the numerical solution of a minimization problem. Since the optimal multipliers are à priori unknown, an algorithm must iterate in both the u-space and in the multiplier space. For equality constraints the optimal solution u^*, η^* constitutes a saddle-point of the Lagrangian [2], and a good initial guess is often required to make the algorithm converge to the optimal solution.

In this section we will specialize to equality constraints $g(u) = 0$. An obvious generalization then is to add the scalar $cg^T(u)g(u)$, where c is a scalar, to the Lagrangian. It is then easy to prove [6] that there exists a $c_0 > 0$, such that for $c \geq c_0$, the function

$$L(u,\eta^*) + cg^T(u)g(u)$$

has a local isolated minimum at $u = u^*$. However, the problem to determine the optimal multipliers η^* still remains.

Next we introduce the concept "Lagrange Multiplier Function" as follows. Let g(u) satisfy the constraint qualifications of lemma 2, and assume that f(u) and g(u) are three times differentiable at u^*. Then the $m \times m$ matrix $\left[g_u g_u^T\right]$ is nonsingular in a neighbourhood of u^*, and the m-dimensional vector

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

is well defined. The conception "multiplier function" is obvious from the following theorem.

Theorem 1

The m-dimensional vector function

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

has the following properties:

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

ii) $\mu(u^*) = \eta^*$

Proof: That $\mu(u)$ is once continuously differentiable follows from the continuity of $\left[g_u g_u^T\right]^{-1}$ and the assumption that f and g are twice continuously differentiable.
The second part of the theorem follows from lemma 1, which states that there exists a unique vector η^* such that $f_u(u^*) + g_u^T(u^*)\eta^* = 0$. Substitute $f_u = - g_u^T\eta^*$ into $\mu(u)$, and it follows that $\mu(u^*) = \eta^*$.

Using the multiplier function, a generalized Lagrangian H(u) is defined.

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

With the assumptions made about f(u) and g(u), H(u) exists and is once continuously differentiable in a neighbourhood of u^*.

Theorem 2

For any value of the real parameter c, the generalized Lagrangian

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

has a stationary point at $u = u^*$.

Proof: A straightforward differentiation of H(u) yields

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

Since $g(u^*) = 0$ and $f_u(u^*) + g_u^T(u^*)\mu(u^*) = f_u(u^*) + g_u^T(u^*)\eta^* = 0$, it follows that $H_u(u^*) = 0$ independent of c.

Intuitively it seems possible that the stationary point $u = u^*$ can now be made a minimum by choosing the value of the parameter c large enough. That this is true is shown in the following theorems.

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 for $c \geq c_0$, $H_u(u^*) = 0$ and $H_{uu}(u^*) \geq 0$.

Proof: In theorem 2 it was shown that $H_u(u^*) = 0$ for any value of the parameter c. To prove the second part of the theorem, $H_{uu}(u)$ is considered.

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

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

which for $u = u^*$ reduces to

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

To compute $\mu_u(u^*)$, $\mu(u)$ is differentiated with respect to u_i.

$$\frac{\partial \mu}{\partial u_i} = \left(g_u g_u^T\right)^{-1} \left(g_{uu_i} g_u^T + g_u g_{uu_i}^T\right) \left(g_u g_u^T\right)^{-1} g_u f_u -$$

$$- \left(g_u g_u^T\right)^{-1} g_{uu_i} f_u - \left(g_u g_u^T\right)^{-1} g_u f_{uu_i} =$$

$$= - \left(g_u g_u^T\right)^{-1} \left[\left(g_{uu_i} g_u^T + g_u g_{uu_i}^T\right) \mu + g_{uu_i} f_u + g_u f_{uu_i}\right]$$

For $u = u^*$, $f_u = - g_u^T \mu$, and

$$\frac{\partial \mu}{\partial u_i} (u^*) = - \left(g_u g_u^T\right)^{-1} g_u \left(g_{uu_i}^T \mu + f_{uu_i}\right)$$

A compact expression for $\mu_u(u^*)$ is then available.

$$\mu_u(u^*) = - \left(g_u g_u^T\right)^{-1} g_u \left(f_{uu} + \sum_{i=1}^{m} \mu^i g^i_{uu}\right)$$

Substitute into H_{uu}.

$$H_{uu}(u^*) = f_{uu} + \sum_{i=1}^{m} \mu^i g^i_{uu} - \left(f_{uu} + \sum_{i=1}^{m} \mu^i g^i_{uu}\right) \cdot$$

$$\cdot\ g_u^T\left(g_u g_u^T\right)^{-1} g_u - g_u^T\left(g_u g_u^T\right)^{-1} g_u \cdot$$

$$\cdot \left(f_{uu} + \sum_{i=1}^{m} \mu^i g^i_{uu}\right) + 2c g_u^T g_u$$

Now let Q be the subspace of R^n spanned by the rows of g_u, and let $Q^\perp$ be the orthogonal complement. If $y_1 \in Q$ and $y_2 \in Q^\perp$, then $y_1^T y_2 = 0$, $g_u y_2 = 0$, and $y_1 = g_u^T \alpha$, where α is uniquely determined by y_1. An arbitrary vector $y \in R^n$ can then be uniquely factorized into $y = y_1 + y_2 = g_u^T\alpha + y_2$, where $y_1 \in Q$ and $y_2 \in Q^\perp$. To prove that $H_{uu}(u^*)$ is positive semidefinite for c sufficiently large, the quantity $y^T H_{uu}(u^*) y$ is considered.

$$y^T H_{uu}(u^*) y = (g_u\alpha + y_2)^T H_{uu}(u^*)(g_u\alpha + y_2) =$$

$$= \alpha^T\left[2c\left(g_u g_u^T\right)\left(g_u g_u^T\right) - g_u\left(f_{uu} + \sum_{i=1}^{m} \mu^i g^i_{uu}\right) g_u^T\right]\alpha +$$

$$+ y_2^T\left(f_{uu} + \sum_{i=1}^{m} \mu^i g^i_{uu}\right) y_2$$

Since $(g_u g_u^T)$ is nonsingular, $2(g_u g_u^T)(g_u g_u^T)$ is positive definite and then there exists a nonsingular matrix T such that

$$2(g_u g_u^T)(g_u g_u^T) = TT^T$$

$$g_u \left(f_{uu} + \sum_{i=1}^{m} \mu^i g_{uu}^i \right) g_u^T = T \begin{bmatrix} \mu_1 & & 0 \\ & \ddots & \\ 0 & & \mu_m \end{bmatrix} T^T$$

Then

$$2c(g_u g_u^T)(g_u g_u^T) - g_u \left(f_{uu} + \sum_{i=1}^{m} \mu^i g_{uu}^i \right) g_u^T > 0$$

for $c > c_0$, where

$$c_0 = \max_i \mu_i$$

According to lemma 3

$$y_2^T \left(f_{uu} + \sum_{i=1}^{m} \mu^i g_{uu}^i \right) y_2 \geq 0$$

since $g_u y_2 = 0$. This finally proves that

$$y^T H_{uu}(u^*) y \geq 0$$

for $c \geq c_0$, and for any $y \in R^n$. Notice that c_0 may be negative.

Theorem 4

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 4 are satisfied. Then there exists a $c_0 > 0$, such that for $c > c_0$, $H_u(u^*) = 0$, and $H_{uu}(u^*) > 0$.

Proof: The proof is identical to the proof of theorem 3, except that strict inequality holds in

$$y_2^T \left(f_{uu} + \sum_{i=1}^{m} \mu^i g_{uu}^i \right) y_2 > 0$$

according to lemma 4. Then there exists c_0, not necessarily positive, such that

$$y^T H_{uu}(u^*) y > 0$$

for $c > c_0$, and for any $y \in R^n$.

For maximum problems, equivalent results are easily obtained by changing the sign of c_0 and c.
Theorems 3 and 4 state the existence of the parameter c_0, and also provide a measure of c_0 when u^* is known. For the numerical computation of u^*, it would, however, be desirable to have an à priori knowledge of a value of c that guarantees that the necessary or sufficient conditions for a minimum of H(u) at u^* are satisfied. This problem will be considered in section 5.

4. INEQUALITY CONSTRAINTS.

If some of the constraints are present as inequalities, $h(u) \leq 0$, a straightforward way to handle them is to introduce slack variables. This could be done in many ways. The most obvious probably is to add the square of a slack variable, i.e.

$$g^i(u) = h^i(u) + v_i^2$$

To simplify the notations it is assumed that just m inequality constraints $h^i(u)$ are present. Further the $(n + m)$-dimensional vector $w^T = (u^T, v_1, \ldots, v_m)$ is introduced as the new variables, and the constraints then are $g^i(w) = 0$, $i = 1, \ldots, m$, where

$$g_w = \left[\begin{array}{c|cccc} & 2v_1 & 0 & \cdots & 0 \\ & 0 & & & \vdots \\ h_u & \vdots & & & 0 \\ & 0 & \cdots & 0 & 2v_m \end{array}\right]$$

If the constraint qualifications hold for those constraints $h^i(u)$ that are active at u^*, i.e. $h^i(u^*)=0$, then $g_w(w^*)$ has rank m, and the equivalent equality constraints also satisfy the constraint qualifications at w^*. Notice, however, that it is not necessary that h_u has rank m. This will for example not be the case for the constraint $a \leq u_i \leq b$ when split up into $h^i(u) = u_i - b \leq 0$ and $h^{i+1}(u) = - u_i - a \leq 0$.

Assume that the constraints $h^1, \ldots, h^\ell$, $\ell \leq m$, are active at u^*, and that $h^{\ell+1}, \ldots, h^m$ are not. To separate active and inactive constraints, the ℓ-dimensional vector $a(u)$ and the $(m - \ell)$-dimensional vector $b(w)$ are introduced.

$$a(u) = \begin{bmatrix} h^1(u) \\ \vdots \\ h^\ell(u) \end{bmatrix} \qquad b(w) = \begin{bmatrix} h^{\ell+1}(u) + v_{\ell+1}^2 \\ \vdots \\ h^m(u) + v_m^2 \end{bmatrix}$$

From lemma 1 it then follows that

$$f_u(u^*) = - a_u^T(u^*)\lambda$$

where λ is an ℓ-dimensional vector consisting of non-negative multipliers $\lambda_1, \ldots, \lambda_\ell$. Similar to section 3, the m-dimensional multiplier function

$$\mu(w) = - \left(g_w g_w^T\right)^{-1} g_w f_w$$

is introduced. As before f(u) and h(u) are assumed to be three times differentiable.

<u>Theorem 5</u>

The multiplier function

$$\mu(w) = - \left(g_w g_w^T\right)^{-1} g_w f_w$$

has the following properties

i) $\mu(w)$ exists and is once continuously differentiable in a neighbourhood of w^*

ii) $\mu^i(w^*) = \lambda_i \qquad i = 1, \ldots, \ell$

$\mu^i(w^*) = 0 \qquad i = \ell+1, \ldots, m$

Proof: To prove the existence of $\mu(w^*)$, it has to be proved that $\left[g_w g_w^T\right]$ is nonsingular at $w = w^*$. Using the notations a(u) and b(w) for active and inactive constraints, $g_w(w^*)$ can be expressed as

$$g_w(w^*) = \left[\begin{array}{c|c|c} a_u & 0 & 0 \\ \hline b_u & 0 & \begin{matrix} 2v_{\ell+1} & & \\ & \ddots & \\ & & 2v_m \end{matrix} \end{array}\right]$$

where all quantities are evaluated at $w = w^*$. Then

$$g_w g_w^T = \left[\begin{array}{c|c} a_u a_u^T & a_u b_u^T \\ \hline b_u a_u^T & b_u b_u^T + V^2 \end{array}\right]$$

where

$$V = \begin{bmatrix} 2v_{\ell+1} & & 0 \\ & \ddots & \\ 0 & & 2v_m \end{bmatrix}$$

V^2 is positive definite since $h^{\ell+1}, \ldots, h^m$ were assumed to be inactive. For the special case where all constraints are active, that is $g_w g_w^T = a_u a_u^T$, the nonsingularity follows from the constraint qualifications. On the other hand, if no constraints are active, $g_w g_w^T = b_u b_u^T + V^2$, and then again $g_w g_w^T$ is nonsingular since V^2 is positive definite. To prove nonsingularity for the general case where some constraints are active and some inactive, the following inversion formula for block matrices is used.

$$\left[\begin{array}{c|c} B_{11} & B_{12} \\ \hline B_{21} & B_{22} \end{array}\right]^{-1} = \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right]$$

where

$$A_{11} = B_{11}^{-1} + B_{11}^{-1} B_{12} B_0^{-1} B_{21} B_{11}^{-1}$$

$$A_{12} = - B_{11}^{-1} B_{12} B_0^{-1}$$

$$A_{21} = - B_0^{-1} B_{21} B_{11}^{-1}$$

$$A_{22} = B_0^{-1}$$

and

$$B_0 = B_{22} - B_{21} B_{11}^{-1} B_{12}$$

Sufficient conditions for the nonsingularity of the block matrix B are thus that B_{11} and B_0 are nonsingular. Substituting $g_w g_w^T$ into the inversion formula, we get

$$A_{11} = (a_u a_u^T)^{-1} + (a_u a_u^T)^{-1} a_u b_u^T X^{-1} b_u a_u^T (a_u a_u^T)^{-1}$$

$$A_{12} = - (a_u a_u^T)^{-1} a_u b_u^T X^{-1}$$

$$A_{21} = - X^{-1} b_u a_u^T (a_u a_u^T)^{-1}$$

$$A_{22} = X^{-1}$$

$$X = b_u b_u^T + V^2 - b_u a_u^T (a_u a_u^T)^{-1} a_u b_u^T =$$

$$= b_u \left\{ I - a_u^T (a_u a_u^T)^{-1} a_u \right\} b_u^T + V^2$$

$(a_u a_u^T)$ is nonsingular since the constraint qualifications were assumed to hold for the active constraints. To prove that X is nonsingular, it is sufficient to prove that $\left\{I - a_u^T(a_u a_u^T)^{-1} a_u\right\}$ is nonnegative definite. Let Q be the ℓ-dimensional subspace of R^n spanned by the rows of a_u, and let $Q^{\perp}$ be the orthogonal complement. Consider the matrix $P = a_u^T(a_u a_u^T)^{-1} a_u$. P takes any vector in Q into itself, because if $x \in Q$, then $x = a_u^T \beta$ and $Px = a_u^T \beta = x$. P also takes any vector in $Q^{\perp}$ into the null vector, because if $y \in Q^{\perp}$, then $a_u y = 0$ and $Py = 0$. Thus P is a projection matrix. Now let $z \in R^n$ be an arbitrary vector. z can uniquely be factorized into $z = x + y$, where $x \in Q$ and $y \in Q^{\perp}$. Then

$$z^T(I - P)z = (x + y)^T(I - P)(x + y) =$$

$$= (x + y)^T(x + y - x) =$$

$$= (x + y)^T y = y^T y \geq 0$$

Thus $\left\{I - a_u^T(a_u a_u^T)^{-1} a_u\right\}$ is nonnegative definite, and X is nonsingular. $(g_w g_w^T)$ is then nonsingular and $\mu(w^*)$ exists. That $\mu(w)$ is once continuously differentiable in a neighbourhood of w^* follows from the continuity of $(g_w g_w^T)^{-1}$, and from the assumptions made about $f(u)$ and $h(u)$.

To prove the second part of the theorem, the relation $f_u(u^*) = - a_u^T(u^*)\lambda$ is used. Then

$$g_w f_w = g_w \begin{bmatrix} f_u \\ \hline 0 \end{bmatrix} = - g_w \begin{bmatrix} a_u^T \\ \hline 0 \end{bmatrix} \lambda = - \begin{bmatrix} a_u a_u^T \\ \hline b_u a_u^T \end{bmatrix} \lambda$$

and

$$\mu(w^*) = \left[\begin{array}{c|c} a_u a_u^T & a_u b_u^T \\ \hline b_u a_u^T & b_u b_u^T + V^2 \end{array}\right]^{-1} \left[\begin{array}{c} a_u a_u^T \\ \hline b_u a_u^T \end{array}\right] \lambda$$

Using the block matrix inversion formula

$$\mu(w^*) = \left[\begin{array}{c} A_{11} a_u a_u^T + A_{12} b_u a_u^T \\ \hline A_{21} a_u a_u^T + A_{22} b_u a_u^T \end{array}\right] \lambda = \left[\begin{array}{c} I_\ell \\ \hline 0 \end{array}\right] \lambda$$

where I_ℓ is the ℓ-dimensional unit matrix. Then $\mu^i(w^*) = \lambda_i$, $i = 1, \ldots, \ell$, and $\mu^i(w^*) = 0$, $i = \ell+1, \ldots, m$.

Similar to section 3 the generalized Lagrangian is now defined as

$$H(w) = f(w) + \mu^T(w)g(w) + cg^T(w)g(w)$$

That the properties of H(w) given by theorems 2 to 4 hold also for the inequality case is shown in the following theorems.

Theorem 6

The generalized Lagrangian

$$H(w) = f(w) + \mu^T(w)g(w) + cg^T(w)g(w)$$

has a stationary point at

$$w^* = \begin{bmatrix} u^* \\ v^* \end{bmatrix}$$

for any value of the real parameter c.

Proof: Differentiate with respect to w.

$$H_w = f_w + g_w^T\mu + \mu_w^T g + 2cg_w^T g = \begin{bmatrix} f_u \\ --- \\ 0 \end{bmatrix} + \begin{bmatrix} a_u^T\lambda \\ --- \\ 0 \end{bmatrix} = 0$$

The last equality follows from lemma 1.

Theorem 7

Let u^* be a local minimum of f(u) subject to the constraints $h(u) \leq 0$. Then there exists c_0, such that for $c \geq c_0$, $H_w(w^*) = 0$ and $H_{ww}(w^*) \geq 0$.

Proof:

$$H_{ww}(w^*) = f_{ww} + \sum_{i=1}^{m} \mu^i g_{ww}^i + \mu_w^T g_w + g_w^T \mu_w + 2cg_w^T g_w$$

$$\mu_w(w^*) = - (g_w g_w^T)^{-1} g_w \left(f_{ww} + \sum_{i=1}^{m} \mu^i g_{ww}^i \right)$$

where all quantities are evaluated at $w = w^*$. For any (n+m)-dimensional vector y_1 such that $y_1 = g_w^T\alpha$, it follows from theorem 3 that $y_1^T H_{ww}(w^*) y_1 > 0$ for $c > c_0$. Then consider $y = y_2$ where $g_w y_2 = 0$. Since f is a function of u only and the slack variables are added as squares, the second derivative matrix $H_{ww}(w^*)$ can be simplified to

$$H_{ww}(w^*) = \left[\begin{array}{c|cccc} f_{uu} + \sum_{i+1}^{\ell} \mu^i g^i_{uu} & & 0 & & \\ \hline & 2\mu^1 & & & \\ 0 & & \ddots & & \\ & & & 2\mu^\ell & \\ & & & & 0 \\ & & & & & 0 \end{array}\right] +$$

$$+ \mu_w^T g_w + g_w^T \mu_w + 2c g_w^T g_w$$

But $g_w y_2 = 0$ implies that $\left[a_u \mid 0\right] y_2 = 0$, and then from lemma 3 and from the fact that $\mu^1, \ldots, \mu^\ell \geq 0$, it follows that $y_2^T H_{ww}(w^*) y_2 \geq 0$, independent of the value of the parameter c.

Theorem 8

Let u^* be a local isolated minimum of f(u) subject to the constraints $h(u) \leq 0$, and assume that the sufficient conditions of lemma 4 are satisfied. Also assume that the multipliers corresponding to the active constraints are strict positive, that is all the active constraints do really affect the solution. Then there exists c_0, such that for $c > c_0$, $H_w(w^*) = 0$ and $H_{ww}(w^*) > 0$.

Proof: It should be proved that $y_2^T H_{ww}(w^*) y_2 > 0$ for any nonzero (n+m)-dimensional vector y_2 such that $g_w y_2 = 0$. Let y_2 be partitioned into

$$y_2^T = \left[y_{21}^T, y_{22}^T, y_{23}^T\right]$$

where y_{21} is an n-dimensional, y_{22} an ℓ-dimensional, and y_{23} an $(m-\ell)$-dimensional vector. Then

$$g_w y_2 = \left[\begin{array}{c} a_u y_{21} \\ \hline b_u y_{21} + V y_{23} \end{array}\right] = 0$$

and

$$y_2^T H_{ww}(w^*) y_2 = y_{21}^T \left(f_{uu} + \sum_{i=1}^{m} \mu^i g_{uu}^i \right) y_{21} +$$

$$+ y_{22}^T \begin{bmatrix} \mu^1 & & \\ & \ddots & \\ & & \mu^\ell \end{bmatrix} y_{22}$$

Thus if $y_{21} \neq 0$ or $y_{22} \neq 0$, $y_2^T H_{ww} y_2 > 0$. Assume that $y_{21} = 0$, $y_{22} = 0$, $y_{23} \neq 0$ and $g_w y_2 = 0$. Then

$$b_u y_{21} + V y_{23} = V y_{23} = 0$$

which, since V is nonsingular, contradicts the assumption that $y_{23} \neq 0$. For every $y_2 \neq 0$, such that $g_w y_2 = 0$, it then follows that $y_2^T H_{ww}(w^*) y_2 > 0$.

5. EXAMPLES AND NUMERICAL CONSIDERATIONS.

The principle of Lagrange multiplier functions will be illustrated in this section with some numerical examples. Aspects on an algorithm for numerical computation will also be briefly discussed.

Consider the problem of minimizing the function

$$f(u) = (u_1 - 5)^2 + (u_2 - 5)^2$$

subject to the equality constraint

$$g^1(u) = (u_2 - 6)^2 - 4(u_1 - 3) = 0$$

The optimal solution is $u_1 = u_2 = 4$.

In fig. 1 contour levels for

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

are drawn for $c = 0.0$ and $c = 0.1$. In the latter case any minimization method should easily find the optimal solution. The example clearly shows the advantage of the method compared with penalty function methods. In these the term $\mu^T(u)g(u)$ is missing, and to reach the optimal solution the parameter c must tend to infinity. The gradient of the function $f(u) + cg^T(u)g(u)$ will then be very large for $g(u) \neq 0$, and even refined minimization methods could get into trouble.

The second example illustrates the slack variable technique to handle inequality constraints. Minimize

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

subject to the constraint

$$h^1(u_1) = u_1 - 1 \leq 0$$

There are two local isolated minima, one at the constraint $u_1 = 1$, and one at $u_1 = -\frac{1}{2}$, where the constraint is not active. The inequality is transformed into an equality constraint by adding the slack variable u_2.

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

Contour levels for H(u) are shown in fig. 2 for c = 0.0, 1.0, 5.0. Since H(u) is symmetric with respect to the u_1 axis, the contour levels are drawn only for $u_2 \geq 0$. The example illustrates the main problem of the method, namely the choice of the parameter c. For c = 1.0, a rather good initial guess of the minimum point is required to get convergence to the optimal solutions, while for c = 5.0 it should be easier to find the solutions. Making c very large, as in the penalty function method, should guarantee convergence in the right directions, but as described above it also destroys the smooth properties of the generalized Lagrangian. A powerful algorithm then should have the possibility to adjust the value of c from a large value at the starting point to a smaller value as the minimum is approached, just to make H(u) as well-conditioned as possible.

Although the slack variable technique increases the order of the system, and for large values of the parameter c creates functions H(u) of the famous Rosenbrock valley type, it can be very useful for problems of smaller dimensions. The method was applied at the following problem [3].

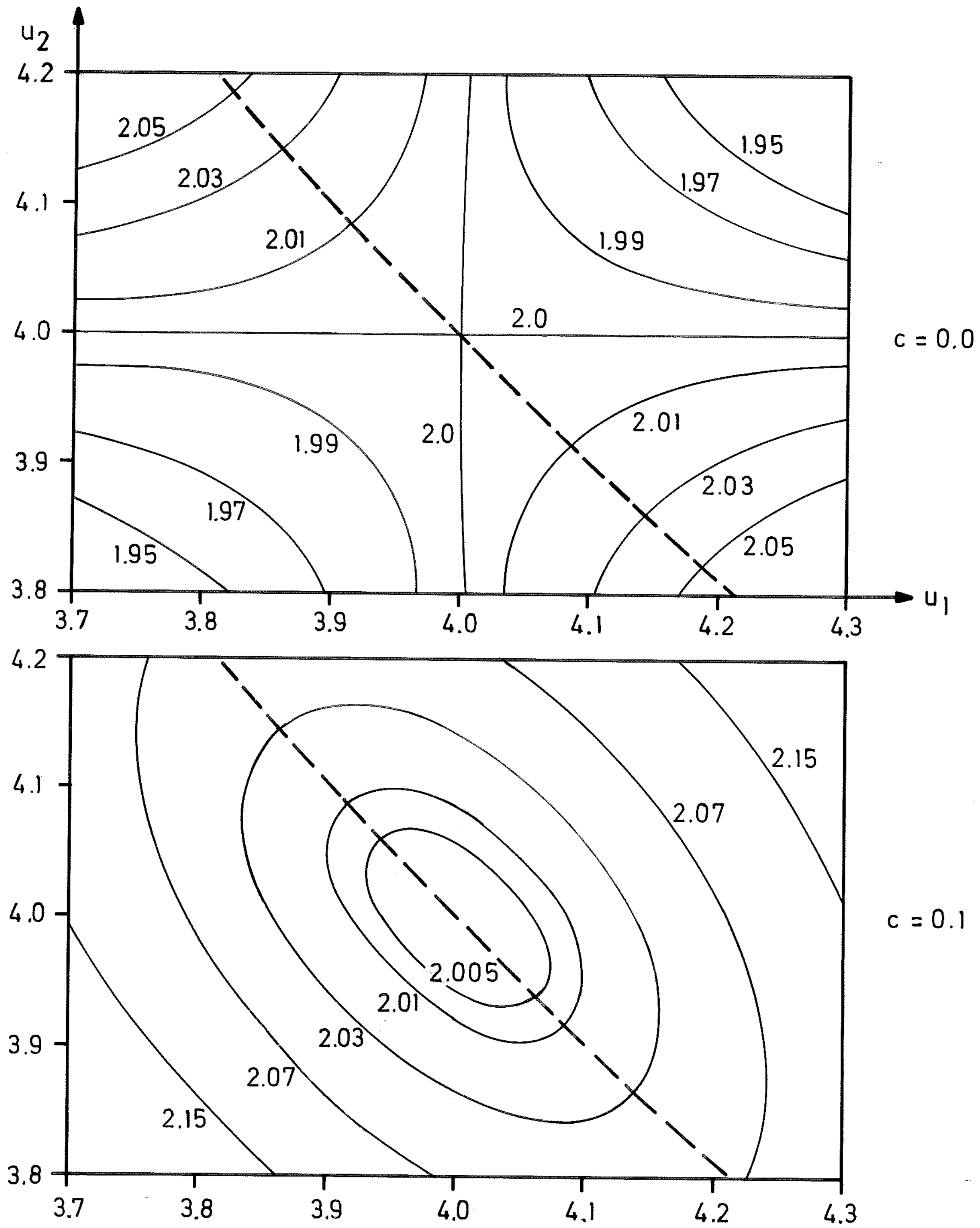

Fig. 1 - Contour levels of the generalized Lagrangian for $f(u) = (u_1-5)^2 + (u_2-5)^2$ and the equality constraint $g(u) = (u_2-6)^2 - 4(u_1-3)$. Contours are drawn for c=0.0 and c=0.1. The dashed line represents the constraint.

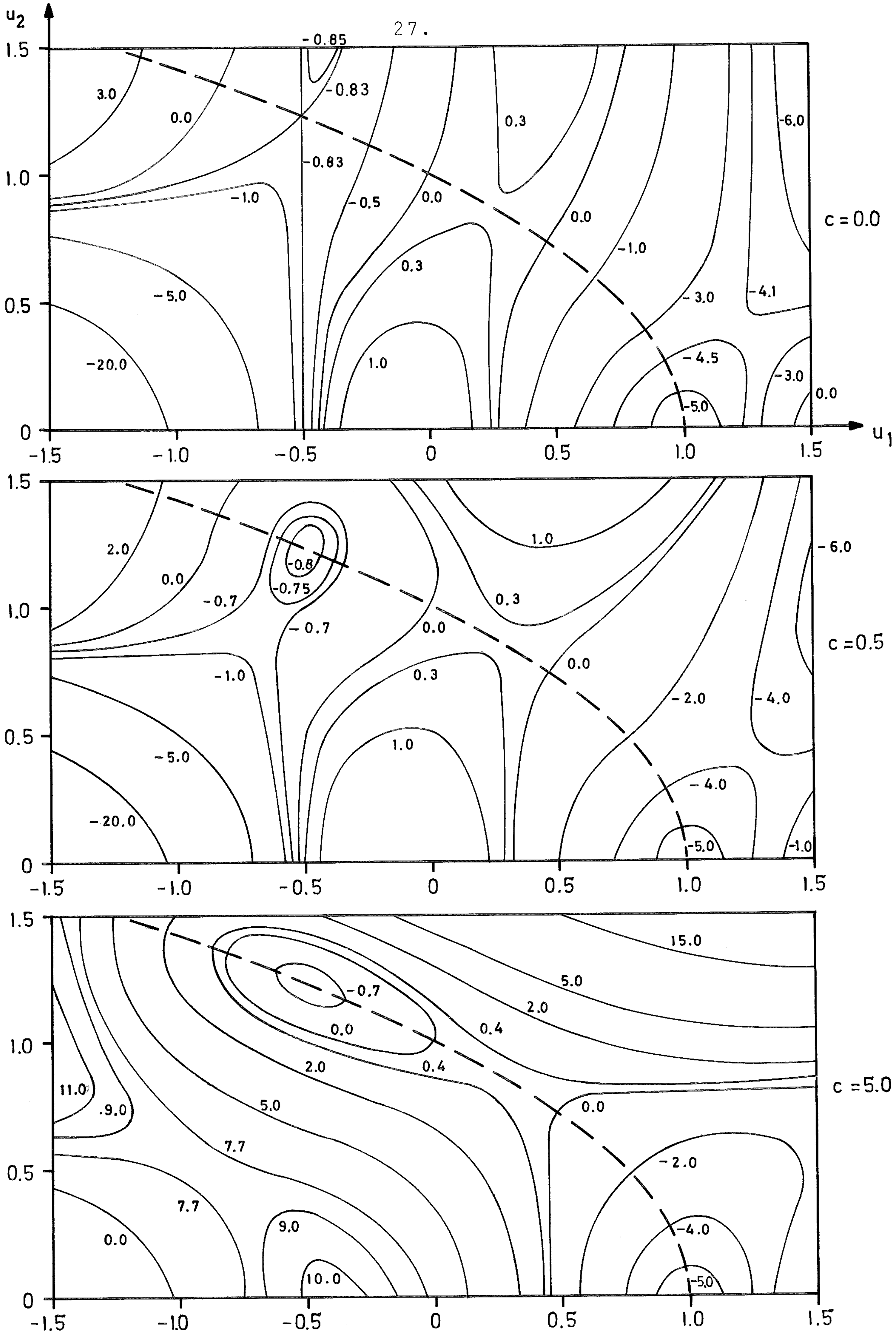

Fig. 2 - Contour levels of the generalized Lagrangian for $f(u) = -\frac{16}{3}u_1^3 - 2u_1^2 + 2u_1$ and the constraint $g(u) = u_1 - 1 + u_2^2 = 0$. Notice that the contours are symmetric with respect to the u_1 axis.

Minimize

$$f(u) = (u_1-u_2)^2 + \left[(u_1+u_2-10)/3\right]^2 + (u_3-5)^2$$

subject to the constraints

$$u_1^2 + u_2^2 + u_3^2 - 48 \leq 0$$

$$-4.5 \leq u_1 \leq 4.5$$

$$-4.5 \leq u_2 \leq 4.5$$

$$-5.0 \leq u_3 \leq 5.0$$

The seven inequality constraints were transformed into equality constraints by introducing slack variables $u_4, \ldots, u_{10}$, and the magnitude of the problem was then very much increased with this brute force approach. Using Powell's minimization method [4], where no gradients are required, the optimal solution was not reached unless the starting point was close to the optimal. The method of Fletcher and Powell [5], which makes use of the gradient, was then chosen. Computation of the gradient

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

then requires the computation of μ_u, which in section 3 was shown to equal

$$\frac{\partial \mu(u)}{\partial u_i} = -(g_u g_u^T)^{-1} \Big[(g_{uu_i} g_u^T + g_u g_{uu_i}^T)\mu + \\ + g_{uu_i} f_u + g_u f_{uu_i} \Big]$$

As initial guess $u_1 = u_2 = u_3 = 0$ was chosen. The slack variables were chosen so that the constraints were approximately satisfied, and the values of the parameter c were c = 1.0, 2.0, 5.0 and 10.0. The optimal solution $u_1 = u_2 = 3.65050$, $u_3 = 4.62036$, corresponding to $f(u^*) = 0.95353$, was found in all cases without any trouble. However, the number of iterations required increased somewhat with increasing value of c. At the optimal solution only the first constraint is active, and a more elaborate algorithm should be able to drop the nonactive constraints, just to keep the dimension of the problem as small as possible.

The expression for c_0 given in theorem 3 is of little value for the à priori estimation of c, since it is difficult to compute the diagonal matrix $\{\mu_i\}$. Moreover, it just describes a local property of the generalized Lagrangian H(u). A more useful estimate is the following. Consider the quantity $g^T(u)g(u)$, which equals zero if and only if the constraints are satisfied. If it is required that

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

the magnitude of $g^T(u)g(u)$ can be decreased by moving in the direction opposite to H_u. Then

$$g^T g_u f_u + g^T g_u \mu_u^T g + g^T g_u g_u^T \mu + 2cg^T g_u g_u^T g > 0$$

which implies

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

for $g(u) \neq 0$. Numerical experiments indicate that this could be useful to estimate a lower bound of the parameter c. For example, consider the point $u_1 = u_2 \cong 3.8$ in fig. 1. For this point the measure yields $c > 0.019$, and thus for $c = 0.020$ $H(u)$ should decrease when moving towards the constraint. This was also confirmed in numerical experiments. However, the parameter value $c = 0.020$ will not cause monotone decrease to the optimal solution, but will create a very flat local minimum in the neighbourhood of $u_1 = u_2 = 3.9$. For this point the c estimate gives $c > 0.021$, which indicates that c should either be chosen well above the limit, for example five or ten times the limit, or there should be possibilities to update c if required.

6. REFERENCES.

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

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

[3] Fletcher, R.: "Optimization", Academic Press, 1969.

[4] Powell, M.J.D.: "An Efficient Method for Finding the Minimum of a Function of Several Variables without Calculating Derivatives", Computer Journal, 7 (1964), pp 155 - 162.

[5] Fletcher, R., and Powell, M.J.D.: "A Rapidly Convergent Descent Method for Minimization", Computer Journal, 6 (1964), pp 163 - 168.

[6] Hestenes, M.R.: "Multiplier and Gradient Methods", Journal of Optimization Theory and Applications, 4 (1969), pp 303 - 320.

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

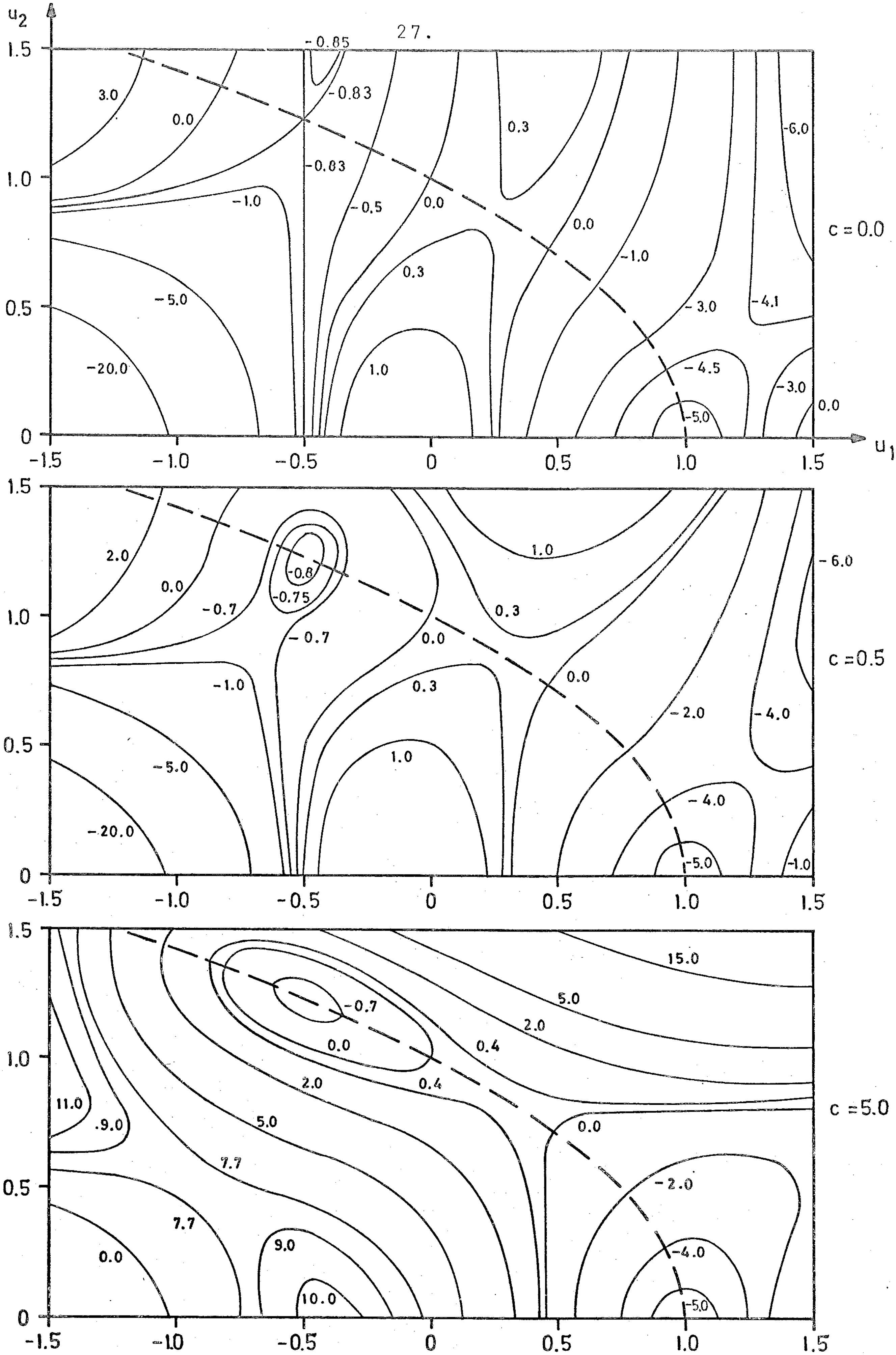

Fig. 2 - Contour levels of the generalized Lagrangian for $f(u) = -\frac{16}{3} u_1^3 - 2u_1^2 + 2u_1$ and the constraint $g(u) = u_1 - 1 + u_2^2 = 0$. Notice that the contours are symmetric with respect to the u_1 axis.

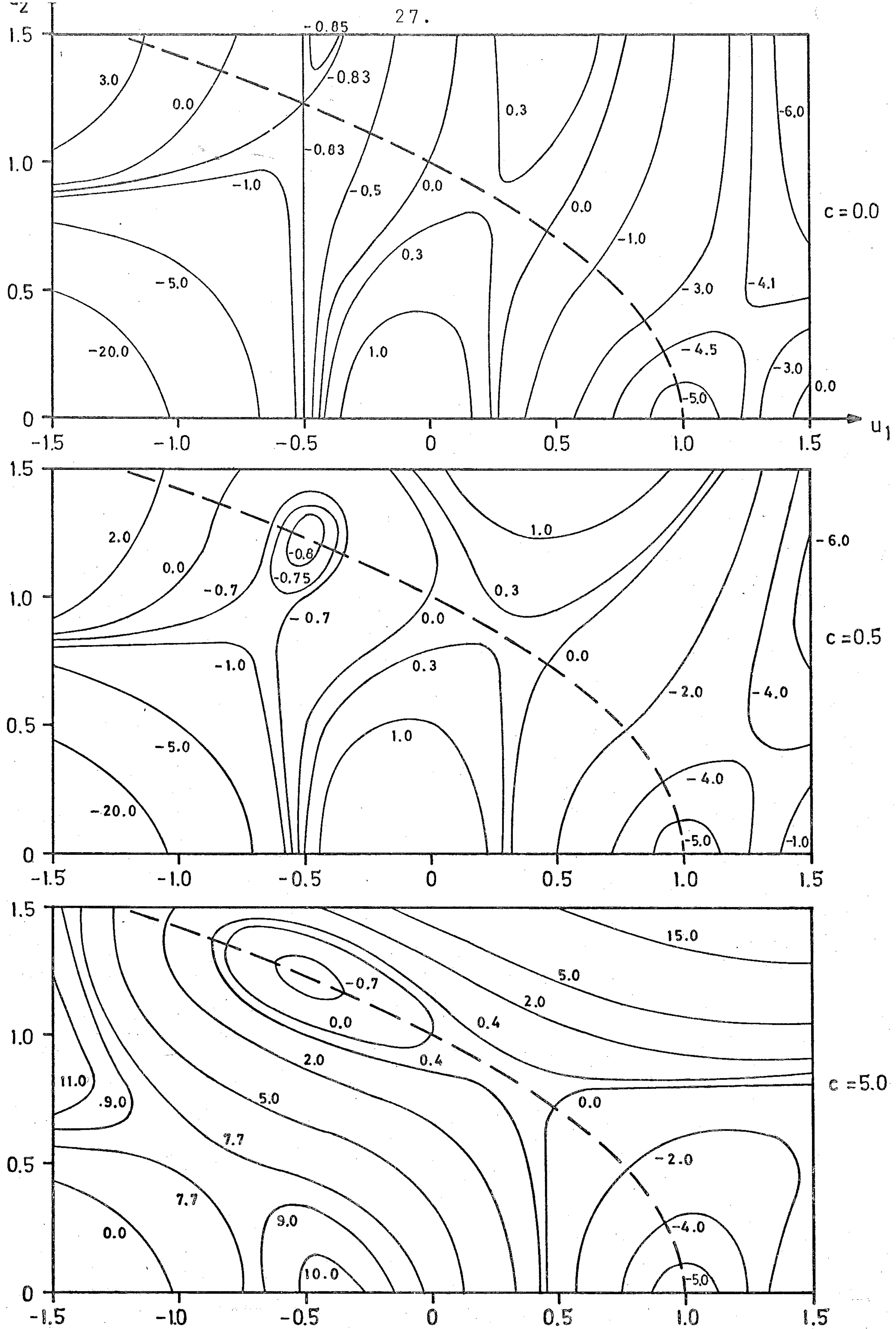

Fig. 2 - Contour levels of the generalized Lagrangian for $f(u) = -\frac{16}{3} u_1^3 - 2u_1^2 + 2u_1$ and the constraint $g(u) = u_1 - 1 + u_2^2 = 0$. Notice that the contours are symmetric with respect to the u_1 axis.