An Introduction to the Algorithms and Theory of Constrained Optimization

Richard Tapia

CRPC-TR90036
1990

Center for Research on Parallel Computation
Rice University
P.O. Box 1892
Houston, TX 77251-1892

AN INTRODUCTION TO THE ALGORITHMS AND THEORY OF CONSTRAINED OPTIMIZATION

R. A. Tapia

1. Introduction and Preliminaries

If $F:R^n \to R^m$, then F_i will denote the i-th component function. $F'(x)$ will denote the Jacobian matrix of F at x and $\nabla F(x)$ denotes $F'(x)^T$ (transpose). In the case that $m=1$, we see that $\nabla F(x)$ will be the gradient of F at x and $\nabla^2 F(x)$ (which with this notation can also be written $\nabla(\nabla F(x))$) will denote the Hessian of F at x. We will have occasion to consider F as a function of two vector variables, say $F(x,\lambda)$. We use the subscript x or λ to denote the partial derivative with respect to x or λ. No subscripts, e.g., $\nabla F(x,\lambda)$ denotes differentiation with respect to the total variable (x,λ). Finally we use the notation $F \in C^k(R^n)$ to mean that F and the partial derivatives of F up to and including order k are continuous. Our presentation of the basic theory will follow Chapter 2 of Fiacco and McCormick (1968).

By the general nonlinear programming problem we mean the constrained optimization problem

$$
\begin{aligned}
(1.1) \qquad & \text{minimize} && f(x) \\
& \text{subject to} && h_i(x)=0, \quad i=1,\dots,p \\
& && g_i(x)\geq 0, \quad i=1,\dots,m
\end{aligned}
$$

where f, g_i, h_i are all defined from R^n into R^1. We will also refer to problem (1.1) as problem (NLP). When each $f, h_i, g_i, \in C^k(R^n)$ we will say <u>problem (NLP) $\in C^k$</u>. In the case that f, h_i and g_i are each <u>linear</u>, i.e., of the form a^Tx+b, we say that problem (NLP) is a <u>linear program</u>. When h_i and g_i are linear and f is <u>quadratic</u>, i.e., $f(x)=a+b^Tx+\frac{1}{2}x^TQx$, where Q is a symmetric $n \times n$ matrix, we say that problem (NLP) is a quadratic program.

Associated with problem (NLP) is the <u>Lagrangian function</u>

$$\ell(x,u,\lambda) = f(x) - \sum_{i=1}^{m} u_i g_i(x) + \sum_{i=1}^{p} \lambda_i h_i(x) \ . \tag{1.2}$$

Observe that $\ell : R^{n+m+p} \to R$. Suppose x satisfies the constraints of problem (NLP) . Let

$$B(x) = \{i : g_i(x) = 0\} \ . \tag{1.3}$$

The equality constraints h_i and the inequality constraints g_i with $i \in B(x)$ are said to be <u>binding</u> or <u>active</u> at x .

The following section will be devoted to the well-known necessity and sufficiency conditions for problem (NLP) . We leave this introductory section by establishing a basic result which will play an important role in the following section.

Lemma (Farkas)

Consider $a_0, a_1, \ldots, a_q \in R^n$. Then the following two statements are equivalent:

i) For all $z \in R^n$ $z^T a_i \geq 0$, $i = 1,\ldots,q$ implies that $z^T a_0 = 0$.

ii) There exist $t_i \geq 0$ such that $a_0 = \sum_{i=1}^{q} t_i a_i$.

<u>Proof</u>. There are several proofs of this lemma in the literature. We will present a proof which is a direct consequence of the duality theorem in linear programming. For other proofs see Mangasarian (1969). Consider the primal linear program

$$\begin{aligned} &\text{minimize} \quad a_0^T z \\ &\text{subject to} \quad A^T z \geq 0 \end{aligned} \tag{1.4}$$

and its dual formulation

$$(1.5)\qquad \begin{aligned} &\text{maximize} \quad 0^T y \\ &\text{subject to} \quad Ay = a_0 \\ &\qquad\qquad\qquad y \geq 0 \end{aligned}$$

where A is the $n \times q$ matrix which has $a_1, \ldots, a_q$ as its columns. Now (i) says that $z = 0$ solves the primal problem. This means that the dual problem must have a feasible point which in turn establishes (ii). The lemma has been established since clearly (ii) implies (i) . ∎

2. Necessity and Sufficiency Conditions for Problem (NLP).

Suppose that problem (NLP) $\in C^1$ and x satisfies the constraints of problem (NLP). Let

$$Z_1(x) = \{z \in R^n : z^T \nabla g_i(x) \geq 0, \quad i \in B(x), \quad z^T \nabla h_i(x) = 0, \quad i=1,\ldots,p \quad \text{and} \quad z^T \nabla f(x) \geq 0\} \tag{2.1}$$

and

$$Z_2(x) = \{z \in R^n : z^T \nabla g_i(x) \geq 0, \quad i \in B(x), \quad z^T \nabla h_i(x) = 0, \quad i = 1,\ldots,p \quad \text{and} \quad z^T \nabla f(x) < 0\} . \tag{2.2}$$

Proposition 2.1. Suppose x^* satisfies the constraints of problem (NLP). Then the following two statements are equivalent:

i) $Z_2(x^*) = \emptyset$

ii) There exists $u^* \in R^m$ and $\lambda^* \in R^p$ such that

$$\nabla_x \ell(x^*,u^*,\lambda^*) = 0 \tag{2.3a}$$

$$g_i(x^*) \geq 0, \quad i = 1,\ldots m \tag{2.3b}$$

$$h_i(x^*) = 0, \quad i = 1,\ldots,p \tag{2.3c}$$

$$u_i^* g_i(x^*) = 0, \quad i = 1,\ldots,m \tag{2.3d}$$

$$u_i^* \geq 0 \quad , \quad i = 1,\ldots,m . \tag{2.3e}$$

Proof. We first show (ii) $\Rightarrow$ (i) . Suppose $z \in Z_2(x^*)$. Then, since $\nabla_x \ell(x^*,u^*,\cancel{w^*}\lambda^*) = 0$ we have

$$0 > z^T \nabla f(x^*) = \sum_{i=1}^{m} u_i^* z^T \nabla g_i(x^*) - \sum_{i=1}^{p} \lambda_i^* z^T \nabla h_i(x^*) . \tag{2.4}$$

But this is a contradiction because each term on the right-hand side of (2.4) is zero. Observe that by (2.3d) $u_i^* = 0$ if $i \notin B(x^*)$.

Let us now establish that (i) $\Rightarrow$ (ii). Suppose that $Z_2(x^*) = \emptyset$. This means that whenever z is such that $z^T\nabla g_i(x^*) \geq 0$, $i \in B(x^*)$, $z^T\nabla h_i(x^*) \geq 0$, $z^T(-\nabla h_i(x^*)) \geq 0$, $i = 1,\ldots,p$ it follows that $z^T\nabla f(x^*) \geq 0$. By the Farkas lemma there exist nonnegative scalars t_i, $i \in B(x^*)$, t_i', t_i'', $i = 1,\ldots,p$ such that

$$\nabla f(x^*) = \sum_{i\in B(x^*)} t_i \nabla g_i(x^*) + \sum_{i=1}^{p} (t_i'\nabla h_i(x^*) - t_i'' \nabla h_i(x^*)) \tag{2.5}$$

In (2.5) let $u_i^* = t_i$, $i \in B(x^*)$ and $u_i^* = 0$ for $i \notin B(x^*)$. Also let $\lambda_i^* = -(t_i' - t_i'')$, $i = 1,\ldots,p$. It now follows that (2.5) can be re-written as $\nabla_x \ell(x^*,u^*,\lambda^*) = 0$. This proves the proposition. ∎

We will refer to conditions (2.3) as the <u>first order conditions</u>. At this point it would be very satisfying if we could say that a necessary condition for x^* to solve problem (NLP) is that $Z_2(x^*) = \emptyset$. This would in turn give the first order conditions (2.3) as necessary conditions. Unfortunately, this statement requires a rather messy qualifier called the constraint qualification. There are numerous constraint qualifications in the literature. The one we present below is one of the most general; others can be found in Mangasarian (1969). We did spend considerable time and effort trying to come up with a constraint qualification which would be less messy, but adequate for the purposes of these rules. However, each attempt led to a theory which was less satisfying. In the study of numerical methods it is appropriate to work with the notion of regularity. Regularity implies our constraint qualification and will be discussed in detail at the end of the present section.

<u>Definition 2.1</u> (Constraint qualification). Suppose that x^* is a feasible point (satisfies the constraints) of problem (NLP). We say that x^* satisfies the <u>weak constraint qualification</u> for problem (NLP) if problem

(NLP) $\in C^1$ and if for each nonzero $z \in R^n$ satisfying

(2.6a) $$z^T \nabla g_i(x^*) \geq 0, \quad i \in B(x^*)$$

(2.6b) $$z^T \nabla h_i(x^*) = 0, \quad i = 1,\ldots,p$$

there exists a $\tau > 0$ and a continuously differentiable arc $A: [0,\tau] \to R^n$ satisfying

(2.7a) $$A(0) = x^*$$

(2.7b) $$A'(0) = z$$

(2.7c) $$g_i(A(t)) \geq 0, \quad t \in [0,\tau), \quad i = 1,\ldots,m$$

(2.7d) $$h_i(A(t)) = 0, \quad t \in [0,\tau), \quad i = 1,\ldots,p \; .$$

Furthermore, we say that the <u>strong constraint qualification</u> for problem (NLP) holds at x^* if the weak constraint qualification holds at x^* and in addition problem (NLP) $\in C^2$, the arc $A \in C^2[0,\tau)$ and for those i's in (2.6a) where equality holds, equality also holds in (2.7c) .

<u>Theorem 2.1</u>. (First Order Necessary Conditions). If x^* satisfies the weak constraint qualification for problem (NLP), then a necessary condition for x^* to be a local solution of problem (NLP) is that $Z_2(x^*) = \emptyset$, or equivalently, that the first order conditions hold.

<u>Proof</u>. Suppose that x^* is a local solution and $z \in Z_2(x^*)$. Clearly $z \neq 0$ so by the weak constraint qualification we have a feasible arc A defined on $[0,\tau)$. For $t > 0$ and small $f(A(t)) - f(A(0)) \geq 0$ so that

$$\frac{f(A(t)) - f(A(0))}{t} \geq 0 \; .$$

This implies that $f'(A(0))A'(0) = z^T \nabla f(x^*) \geq 0$ which is a contradiction. ∎

<u>Theorem 2.2</u>. (First Order and Second Order Necessary Conditions). If x^* satisfies the strong constraint qualification for problem (NLP), then,

necessary conditions for x^* to be a local solution of problem (NLP) are:

There exist $u^* \in R^m$ and $\lambda^* \in R^p$ satisfying

(2.8a) $$\nabla_x \ell(x^*, u^*, \lambda^*) = 0$$

(2.8b) $$g_i(x^*) \geq 0, \quad i = 1,\dots,m$$

(2.8c) $$h_i(x^*) = 0, \quad i = 1,\dots,p$$

(2.8d) $$u_i^* g_i(x^*) = 0, \quad i = 1,\dots,m$$
$$u_i^* \geq 0, \quad i = 1,\dots,m$$

and

(2.9) $$z^T \nabla_x^2 \ell(x^*, u^*, \lambda^*) z \geq 0$$

whenever

(2.10a) $$z^T \nabla g_i(x^*) = 0, \quad i \in B(x^*)$$

(2.10b) $$z^T \nabla h_i(x^*) = 0, \quad i = 1,\dots,p \ .$$

Proof. Conditions (2.8) are merely a restatement of Theorem 2.1. We now restrict our attention to the second order necessary condition (2.9) . Let A be the arc guaranteed by the strong constraint qualification and let

(2.11) $$\Phi(t) = \ell(A(t), u^*, \lambda^*) \qquad t \in [0, \tau) \ .$$

where ℓ is given in (1.2). From the fact that x^* is a local solution of problem (NLP) and the strong constraint qualification it follows that $t = 0$ is a minimizer of Φ . Also

(2.12) $$\Phi_+'(t) = \nabla_x \ell(A(t), u^*, \lambda^*) A'(t)_+$$

so $\Phi_+'(0) = 0$. It follows that $\Phi_+''(0) \geq 0$.

But

(2.13) $$\Phi_+''(0) = z^T \nabla_x^2 \ell(x^*, u^*, \lambda^*) z + \nabla_x \ell(x^*, u^*, \lambda^*) A_+''(0).$$

The theorem now follows since the second term on the right-hand side of (2.13) is zero. ∎

Theorem 2.3. (Sufficiency Conditions). Suppose problem (NLP) $\in C^2$. Then sufficient conditions that x^* be an isolated (unique locally) local solution of problem (NLP) are:

There exist $u^* \in R^m$ and $\lambda^* \in R^p$ satisfying

(2.14a) $$\nabla_x \ell(x^*, u^*, \lambda^*) = 0$$

(2.14b) $$g_i(x^*) \geq 0, \quad i = 1,\ldots,m$$

(2.14c) $$h_i(x^*) = 0, \quad i = 1,\ldots,p$$

(2.14d) $$u_i^* g_i(x^*) = 0, \quad i = 1,\ldots,m$$

(2.14e) $$u_i^* = 0, \quad i = 1,\ldots,m$$

and for every nonzero $z \in R^n$ satisfying

(2.15a) $$z^T \nabla g_i(x^*) = 0, \quad i \in D^* = \{i : u_i^* > 0\}$$

(2.15b) $$z^T \nabla g_i(x^*) \geq 0, \quad i \in B(x^*) - D^*$$

(2.15c) $$z^T \nabla h_i(x^*) = 0, \quad i = 1,\ldots,p$$

we have that

(2.16) $$z^T \nabla_x^2 \ell(x^*, u^*, \lambda^*) z > 0 \ .$$

Proof. Suppose x^* satisfies the above conditions and it is not a local solution of problem (NLP). Then there exists $\{y^k\}$ such that

(2.17a) $$y^k \neq x^*$$

(2.17b) $$y^k \to x^*$$

(2.17c) $$y^k \text{ is feasible}$$

(2.17d) $$f(y^k) \leq f(x^*) \ .$$

Let $\delta_k = \|y^k - x^*\|$ and $s_k = (y^k - x^*)/\|y^k - x^*\|$, so that $y^k = x^* + \delta_k s_k$. Notice that $0 < \delta_k \to 0$ and $\|s_k\| = 1$. Let $(0, \bar{s})$ be an accumulation point of the sequence $\{(\delta_k, s_k)\}$. Without any loss of generality we may assume that $(\delta_k, s_k) \rightarrow (0, \bar{s})$. We will now show that $z = \bar{s}$ satisfies conditions (2.15a)-(2.15c). Now recalling that $y^k = x^* + \delta_k s_k$ we have that

$$(2.18) \qquad g_i(x^* + \delta_k s_k) - g_i(x^*) \geq 0, \quad i \in B(x^*)$$

$$(2.19) \qquad h_i(x^* + \delta_k s_k) - h_i(x^*) = 0, \quad i = 1, \ldots, p$$

$$(2.20) \qquad f(x^* + \delta_k s_k) - f(x^*) \leq 0 \ .$$

Dividing (2.18), (2.19) and (2.20) by δ_k and letting $k \rightarrow \infty$ we obtain

$$(2.21) \qquad \bar{s}^T \nabla g_i(x^*) \geq 0, \quad i \in B(x^*)$$

$$(2.22) \qquad \bar{s}^T \nabla h_i(x^*) = 0, \quad i = 1, \ldots, p$$

$$(2.23) \qquad \bar{s}^T \nabla f(x^*) \leq 0 \ .$$

Now, from (2.14a) and (2.21) we have

$$(2.24) \qquad 0 \geq \bar{s}^T \nabla f(x^*) = \sum_{i \in D^*} u_i^* \bar{s}^T \nabla g_i(x^*) - \sum_{i=1}^{p} \lambda_i^* \bar{s}^T \nabla h_i(x^*)$$

Equation (2.22) shows that the last sum in (2.24) is zero. From (2.14c) and (2.21) it follows that (2.24) leads to a contradiction if we have strict inequality in (2.21) for any $i \in D^*$. It therefore follows that for $i \in D^*$ we must have $s^T \nabla g_i(x^*) = 0$. We have established that $\bar{s}$ satisfies (2.15a) - (2.15c). Since $y^k = x^* + \delta_k D_k$ we can use Taylor's theorem to expand about the point x^k, i.e.,

$$(2.25) \qquad 0 \leq g_i(y^k) = g_i(x^*) + \delta_k s_k^T \nabla g_i(x^*) + \frac{\delta_k^2}{2} s_k^T \nabla^2 g_i(x^* + \theta_i \delta_k s_k) s_k$$

$$(2.26) \qquad 0 = h_i(y^k) = h_i(x^*) + \delta_k s_k^T \nabla h_i(x^*) + \frac{\delta_k^2}{2} s_k^2 \nabla^2 h_i(x^* + \mu_i \delta_k s_k) s_k$$

$$(2.27) \qquad 0 \geq f(y^k) - f(x^*) = \delta_k s_k^T \nabla f(x^*) + \frac{\delta_k^2}{2} s_k^T \nabla^2 f(x^* + \theta_0 \delta_k s_k) s_k \ .$$

Multiplying (2.25) by $-u_i^*$, (2.26) by λ_i^* and then adding and summing on i leads to

$$0 \geq \delta_k s_k^T \nabla_x \ell(x^*, u^*, \lambda^*) + \frac{\delta_k^2}{2} s_k^T A s_k \tag{2.28}$$

where

$$A = \nabla^2 f(x^* + \theta_0 \delta_k D_k) - \sum_{i=1}^{m} u_i^* \nabla^2 g_i(x^* + \theta_i \delta_k s_k) + \sum_{i=1}^{p} \lambda_i^* \nabla^2 h_i(x + \mu_i \delta_k s_k) \tag{2.29}$$

Observe that the first term on the right-hand side of (2.28) is equal to zero. Divide (2.28) by δ_k^2 and let $k \to \infty$ to obtain

$$0 \geq \bar{s}^T \nabla_x^2 \ell(x^*, u^*, \lambda^*) \bar{s} \ . \tag{2.30}$$

But (2.30) contradicts (2.16) since we have already established that $\bar{s}$ satisfies (2.15a) - (2.15c). ∎

<u>Definition 2.2</u>. (Regularity). Suppose that problem (NLP) $\in C^1$. Then the feasible point $x \in R^n$ is said to be a <u>regular</u> point of problem (NLP) if

$$\{\nabla h_1(x), \ldots, \nabla h_p(x), \nabla g_i(x), \quad i \in B(x)\} \tag{2.31}$$

is a linearly independent set.

Many of our numerical algorithms require regularity. It is indeed fortunate then that regularity implies our constraint qualification.

<u>Theorem 2.3</u> (Regularity). Let x be a regular and feasible point of problem (NLP). If problem (NLP) $\in C^1$, then x satisfies the weak constraint qualification. If, in addition, problem (NLP) $\in C^2$, then x also satisfies the strong constraint qualification.

<u>Proof</u>. Let nonzero $z \in R^n$ be such that

$$z^T \nabla g_i(x) \geq 0, \quad i \in B(x) \tag{2.32a}$$

$$z^T \nabla h_i(x) = 0, \quad i = 1, \ldots, p \ . \tag{2.32b}$$

Now, if there are no equality constraints and $z^T \nabla g_i(x) > 0 \ \forall \ i \in B(x)$, then clearly

$$A(t) = x + tz$$

is feasible for t small and positive. So, let us consider

(2.33) $$G(x) = [g_{i_1}(x),\ldots,g_{i_s}(x),h_1(x),\ldots,h_p(x)]$$

where $\{i_1,\ldots,i_s\} = \{i \in B(x): z^T \nabla g_i(x) = 0\}$.

We have

(2.34) $$\nabla G(x) = [\nabla g_{i_1},\ldots,g_{i_s}(x),\nabla h_1(x),\ldots,\nabla h_p(x)]$$

and $\nabla G(x)$ is an n by $(s+p)$ matrix where $(s+p) < n$. By regularity $\nabla G(x)$ has linearly independent columns, so we may consider

$$[\nabla G(x)^T]^+ = \nabla G(x)[\nabla G(x)^T \nabla G(x)]^{-1} .$$

Then

(2.35) $$\{I - [\nabla G(x)^T]^+ \nabla G(x)^T\}z = z$$

since $\nabla G(x)^T z = 0$. Consider the initial value problem

(2.36a) $$A'(t) = [I - \nabla G(A(t))[\nabla G(A(t))]^{-1} \nabla G(A(t))^T]z$$

(2.36b) $$A(0) = x .$$

From ordinary differential equation theory, the IVP (2.36) has a solution $A(t)$ on $[0,\tau)$ for some $\tau > 0$. Moreover, from (2.36a) $A'(0) = z$, and $A \in C^1$ if problem (NLP) $\in C^1$ and $A \in C^2$ if problem (NLP) $\in C^2$. We will have established the theorem as soon as we show that $A(t)$ is feasible on a small interval.

For $i \notin B(x)$ we see that $g_i(A(t)) > 0$ for small positive t . Also, for $i \in B(x)$ such that $z^T \nabla g_i(x) > 0$ we will have $g_i(A(t)) > 0$ for small positive t . We need only look at the constraints included in G defined by (2.23). For the sake of simplicity denote $G = [G_1,\ldots,G_{0+p}]$.

From Taylor's theorem for $t < \tau$ and $k = 1,\ldots,s+p$

(2.37) $$G_k(A(t)) = G_k(A(0)) + \nabla G_k(A(\theta_k))^T A'(\theta_k), \quad 0 < \theta_k < t .$$

From (2.36a) we see that

$$(2.38) \qquad \nabla G(A(\theta_k))^T A'(\theta_k) = 0 \quad \text{for any} \quad 0 < \theta_k < t \ .$$

It follows from (2.37) and (2.38) that

$$(2.39) \qquad G_k(A(t)) = 0, \quad k = 1,\ldots,s+p \quad \text{and} \quad 0 \le t < \tau \ .$$

It is exactly (2.39) that says the strong constraint qualification holds. ∎

3. Quasi-Newton Methods and the Fundamental Extended Problem. By a quasi-Newton method for approximating a stationary point x^* of $f:R^n \to R$ (i.e., $\nabla f(x^*) = 0$) we mean the iterative procedure

$$\bar{x} = x - \alpha B^{-1}\nabla f(x), \quad 0 < \alpha \leq 1 \tag{3.1}$$

$$\bar{B} = \mathcal{B}(x,\bar{x},B) \ . \tag{3.2}$$

The matrix $\mathcal{B}(x,\bar{x},B)$ is interpreted as an approximation to $\nabla^2 f(x^*)$. There are several philosophies for choosing the scalar α in (3.1). One popular approach is the so-called line search. Namely, if one is attempting to approximate a minimizer of f, then α is chosen as an approximation to the solution of the one-dimensional minimization problem.

$$\text{minimize } f(x - \alpha\nabla f(x)), \quad \alpha \geq 0 \ . \tag{3.3}$$

If one is attempting to approximate a maximizer of f, then (3.3) is replaced with

$$\text{maximize } f(x - \alpha\nabla f(x)), \quad \alpha \geq 0 \tag{3.4}$$

and if one is attempting to approximate only a stationary point of f, then one could replace (3.3) with

$$\text{minimize } \|\nabla f(x - \alpha\nabla f(x))\|^2, \quad \alpha \geq 0 \ .$$

The choice of α is often referred to as step length control and plays an important role in the global behavior of the algorithm.

Four popular quasi-Newton methods are

The Gradient Method:

$$\mathcal{B}(x,\bar{x},B) = I \tag{3.5}$$

Newton's Method:

$$\mathcal{B}(x,\bar{x},B) = \nabla^2 f(\bar{x}) \ . \tag{3.6}$$

Finite Difference Newton's Method:

$$(3.7) \qquad \mathcal{B}(x,\bar{x},B) = \left(\frac{1}{h}\left[\frac{\partial f(\bar{x}+he_j)}{\partial x_i} - \frac{\partial f(\bar{x})}{\partial x_i}\right]\right)$$

where $e_1,\ldots,e_n$ are the natural basis vectors for R^n, h is a small positive scalar, and (a_{ij}) denotes the matrix whose i,j-th component is a_{ij} .

Secant Methods:

$$(3.8) \qquad \mathcal{B}(x,\bar{x},B) = \mathcal{B}_S(s,y,B)$$

where $s = \bar{x} - x$, $y = \nabla f(\bar{x}) - \nabla f(x)$ and $\mathcal{B}_S$ satisfies the secant equation

$$(3.9) \qquad \mathcal{B}_S(s,y,B)s = y \ .$$

At the present time the most popular secant update is the BFGS given by

$$(3.10) \qquad \bar{B} = B + yy^T/y^Ts - Bss^TB/s^TBs$$

and in inverse form by

$$(3.11) \qquad \bar{H} = H - [sy^TH + (Hy - s)s^T]/s^Ty + ss^T(y^THy/s^Ty)^2$$

where $H = B^{-1}$ and $\bar{H} = \bar{B}^{-1}$. For more detail, see Dennis and Moré (1977).

Let us consider the special case of problem (NLP) (see 1.1), where we only have equality constraints. Namely,

$$(3.12) \qquad \text{minimize } f(x)$$

$$\text{subject to} \qquad h_i(x) = 0, \quad i = 1,\ldots,p \ .$$

We will also refer to problem (3.12) as problem (EQ). Suppose problem (EQ) $\in C^2$. Let x^* be a local solution which is also a regular point. The first order necessary conditions (see Theorem 2.1) and regularity (see Theorem 2.3) imply that there exists a Lagrange multiplier λ^* such that (x^*,λ^*) is a solution of the nonlinear system

$$(3.13) \qquad \nabla \ell(x,\lambda) = 0$$

Observe that

$$\nabla \ell(x,\lambda) \equiv \begin{pmatrix} \nabla_x \ell(x,\lambda) \\ \\ \nabla_\lambda \ell(x,\lambda) \end{pmatrix} = \begin{pmatrix} \nabla f(x) + \nabla h(x)\lambda \\ \\ h(x) \end{pmatrix} \tag{3.14}$$

and

$$\nabla^2 \ell(x,\lambda) = \begin{pmatrix} \nabla_x^2 \ell(x,\lambda) & \nabla h(x) \\ \\ \nabla h(x)^T & 0 \end{pmatrix} . \tag{3.15}$$

By the <u>extended problem</u> corresponding to problem (EQ) we mean problem (3.13). In other words, by the extended problem we mean the problem of finding a stationary point of the Lagrangian functional. Moreover, it is also classical that (x^*, λ^*) corresponds to a saddle point of the extended problem. Indeed, under the assumption of regularity we have that $\nabla h(x^*) \neq 0$ and it is not difficult to demonstrate that this implies that $\nabla^2 \ell(x^*, \lambda^*)$ is necessarily indefinite and the saddle point behavior follows. The motivation for our use of the terminology 'extended' should be clear from the fact that the dimension of problem (3.12) (i.e., number of independent variables) is $n + p$.

The extended problem will play a fundamental role in our development and actually has been in the background of the derivation of many algorithms whether the researcher was aware of it or not. Our basic assumptions for much of the analysis given in this paper will be the standard Newton's method assumptions for the extended problem. Specifically, we assume

(3.16) (i) f and h have three continuous derivatives

and

(3.17) (ii) $\nabla^2 \ell(x^*, \lambda^*)$ is invertible.

The latter assumption (ii) is often referred to as <u>nonsingularity</u> of the solution x^* and clearly implies the regularity of x^* (see proposition 3.1).

Before we move on we would like to make some observations concerning the historical development of algorithms for constrained minimization problems. Initially there was an excessive amount of effort spent on attacking the constrained minimization problem by solving a sequence of unconstrained minimization problems. These approaches were usually rationalized by arguing that in this way one is able to utilize the excellent new quasi-Newton algorithms for unconstrained minimization. Specifically, we first witnessed considerable activity in penalty function methods and then substantial activity in multiplier methods. In our opinion this philosophy retarded the progress of constrained optimization theory. Fortunately, we have finally arrived at the point where workers in the area of constrained optimization are no longer wearing the straightjacket of sequential unconstrained minimization formulations. The penalty function method and the multiplier method played an important role in the molding and development of contemporary thought and as such will be discussed in detail in the following section.

A main point of the present section is that the entire course of events, including the recent activity in the area of quasi-Newton methods for constrained minimization, can be explained best in terms of the extended problem. To begin with, quasi-Newton methods are, in their purest form, algorithms for solving systems of nonlinear equations. This means that with respect to nonlinear functionals they are algorithms for approximating stationary points and not necessarily just minimizers or maximizers. Indeed, this is the way they were presented earlier in this section. However, many researchers seem to be secure only when they are applying these algorithms to a minimization (or maximization) problem, and the vast majority of research activity in constrained optimization has historically ignored the extended problem. The truly fascinating aspect of this research area is that (without being aware of it) researchers have very recently suggested quasi-Newton methods for constrained optimization problems which can be shown to be equivalent to a quasi-Newton method applied to the extended problem. Two of the more popular approaches will be discussed in detail in Sections 7 and 8. In summary, it is interesting that the circle has been completed and we are now at a point in the development of the theory that we would have been ten years ago, had it not been for the sequential unconstrained minimization detour.

By a structured quasi-Newton method for the extended problem we mean the iterative procedure

$$\begin{pmatrix}\bar{x}\\ \bar{\lambda}\end{pmatrix} = \begin{pmatrix}x\\ \lambda\end{pmatrix} - B^{-1}\nabla \ell(x,\lambda) \tag{3.17}$$

$$\bar{B} = \begin{bmatrix}\bar{B}_x & \nabla g(\bar{x})\\ \nabla h(\bar{x})^T & 0\end{bmatrix} \tag{3.18}$$

where $\bar{B}_x$ is an approximation to $\nabla_x^2 \ell(x^*,\lambda^*)$.

We use the adjective structured to mean that we don't approximate the complete matrix $\nabla^2 \ell(x,\lambda)$ (see (3.14)) but only the part which contains second order information, namely, the upper left-hand corner $\nabla_x^2 \ell(x,\lambda)$. A general quasi-Newton method for the extended problem could approximate all of $\nabla^2 \ell(x,\lambda)$.

The structured secant methods result by choosing

$$\bar{B}_x = \mathcal{B}_S(s,y,B_x) \tag{3.19}$$

where $s = \bar{x} - x$, $y = \nabla_x \ell(\bar{x},\bar{\lambda}) - \nabla_x \ell(x,\bar{\lambda})$, B_x is the current approximation to $\nabla_x^2 \lambda(x^*,\lambda^*)$ and $\mathcal{B}_S$ is one of the popular secant updates.

It should be clear that Newton's method for the extended problem and the structured Newton method (i.e., in (3.19) $\bar{B}_x = \nabla_x^2 \ell(\bar{x},\bar{\lambda})$) are the same, consequently the adjective structured in this case is redundant. It follows that the convergence analysis for the structured Newton method is the standard theory. In particular, assuming the standard conditions (3.16) and (3.17), we will have local Q-quadratic convergence in the variable (x,λ) .

The matrix $\nabla^2 \ell(x,\lambda)$ given by (3.15) is never positive definite. Consequently the BFGS secant method cannot be applied directly to the extended problem. However, the matrix $\nabla_x^2 \ell(x,\lambda)$ is often positive definite, hence, in this case the structured BFGS secant method for the extended problem makes sense. In fact, the following convergence analysis has been established by Tapia (1977).

<u>Theorem 3.1</u>. Let x^* be a local solution of problem (EQ). Assume that the standard conditions (3.16) and (3.17) hold and that $\nabla_x^2 \ell(x^*,\lambda^*)$ is positive definite. Then the structured BFGS secant method is locally Q-superlinearly convergent in the variable (x,λ) .

We leave this section by analyzing the close interaction between nonsingularity, and regularity. For the remaining results we shall assume that problem (EQ) $\in C^2$.

<u>Proposition 3.1</u>. Consider the following statements:

(i) x^* is a nonsingular point of problem (EQ)

(ii) x^* is a regular point of problem (EQ)

(iii) If x^* is a local solution of problem (EQ), then there exists a unique multiplier λ^* satisfying $\nabla_x \ell(x^*,\lambda^*) = 0$.

Then (i) $\Rightarrow$ (ii) $\Rightarrow$ (iii) .

<u>Proof</u>. The proof is direct and straightforward.

Proposition 3.2. Let x^* be a local solution of problem (EQ) which is also a regular point. Then x^* is a nonsingular point if and only if $\nabla_x^2 \ell(x^*,\lambda^*)$ is positive definite on the linear subspace

$$\{V: \nabla h_i(x^*)^T V = 0, \quad i = 1,\ldots,p\} \quad . \tag{3.20}$$

Proof. The proof will follow directly from the following lemma.

Lemma 3.1. Suppose that A is an $n \times n$ symmetric matrix and H is an $n \times p$ matrix of rank p such that

$$V^T A V \geq 0$$

for all $V \in R^n$ satisfying

$$H^T V = 0 \ .$$

Then $V^T A V > 0 \ \ \forall V \neq 0$ if and only if the matrix

$$\begin{pmatrix} A & H \\ H^T & 0 \end{pmatrix} \tag{3.21}$$

is nonsingular.

Proof. Our proof follows Buys (1972). Suppose that A is not positive definite on the subspace (3.20). Then there exists $V_0 \neq 0$ such that

$$V_0^T A V_0 = 0$$

and

$$H^T V_0 = 0 \quad .$$

The constrained optimization problem

$$\text{minimize } \{\tfrac{1}{2} V^T A V : H^T V = 0\}$$

is solved by V_0. So there exists $u_o \in R^p$ satisfying

$$AV_0 + Hu_0 = 0 \ ; \tag{3.22}$$

equivalently

$$\begin{pmatrix} A & H \\ H^T & 0 \end{pmatrix} \begin{pmatrix} V_0 \\ u_0 \end{pmatrix} = 0 \ .$$

This gives a contradiction.

Now suppose that the matrix (3.21) is singular. There exist vectors $V_0 \in R^n$ and $u_0 \in R^p$, not both zero, such that (3.22) holds. If $V_0 = 0$, then $Hu_0 = 0$, but H has full rank, so $u_0 = 0$. Hence we must have $V_0 \neq 0$ and

$$V_0^T A V_0 = -V_0^T H u_0 = 0 \ .$$

This proves the lemma. ■

Corollary 3.1. Any nonsingular point x^* which satisfies the first and second order necessary conditions (Theorem 1.2) also satisfies the sufficiency conditions (Theorem 1.3).

Corollary 3.2. Any regular point which satisfies the second order sufficiency conditions (Theorem 1.3) is a nonsingular point.

4. Penalty Function Methods. We begin by considering problem (EQ) given in (3.12). If we let $h(x) = (h_1(x),\dots,h_p(x))$ then the classical Lagrangian for this problem as given by (1.2) is $\ell(x,\lambda) = f(x) + \lambda^T h(x)$.

In the penalty function method and the multiplier method we will be concerned with the sequential minimization of the following two functionals.

Penalty Function for Problem (EQ).

$$P(x;C) = f(x) + \tfrac{1}{2}Ch(x)^T h(x) \qquad (C > 0) \tag{4.1}$$

and

Augmented Lagrangian Function for Problem (EQ)

(4.2) $$L(x,\lambda;C) = f(x) + \lambda^T h(x) + \tfrac{1}{2}Ch(x)^T h(x) \qquad (C \geq 0) \ .$$

The semicolon in front of the penalty constant C in (4.1) and (4.2) is used to denote the fact that C will be treated as a parameter and not an independent variable. In particular, we will never differentiate with respect to C .

A fundamental question is whether the functionals $p(x;C)$ and $L(x,\lambda;C)$ have minimizers in x for a fixed C and a fixed λ .

Straightforward calculations give

(4.3) $$\nabla_x^2 \ell(x,\lambda) = \nabla^2 f(x) + \lambda_1 \nabla^2 h_1(x) + \ldots + \lambda_m \nabla^2 h_m(x) ,$$

(4.4) $$\nabla^2 P(x;C) = \nabla_x^2 \ell(x, Ch(x)) + C\nabla h(x) \nabla h(x)^T \ ,$$

and

(4.5) $$\nabla_x^2 L(x,\lambda;C) = \nabla_x^2 \ell(x, \lambda + Ch(x)) + C\nabla h(x) \nabla h(x)^T \ .$$

Let x^* be a local solution of problem (EQ) and λ^* its associated multiplier. It is known that $\nabla_x^2 \ell(x^*,\lambda^*)$ may be indefinite; hence the Lagrangian functional $\ell(x,\lambda^*)$ need not have a minimizer in x . However, the following theorem shows that for C sufficiently large, the Hessian of the augmented Lagrangian functional at (x^*,λ^*) is positive definite. This means that the penalty functional will have a local minimizer in x provided $Ch(x)$ is near λ^*, while the augmented Lagrangian will have a minimizer in x provided $\lambda + Ch(x)$ is near λ^* .

Theorem 4.1. Let x^* be a local solution of problem (EQ) and let λ^* be its associated multiplier. Suppose that the standard conditions (3.16) and (3.17) hold. Then there exists $\hat{C} > 0$ such that for all $C \geq \hat{C}$ the matrix

(4.6) $$\nabla_x^2 \ell(x^*,\lambda^*) + C\nabla h(x^*)\nabla h(x^*)^T$$

is positive definite.

<u>Proof</u>. We give a short proof due to Buys (1972). Let A denote $\nabla_x^2 \ell(x^*,\lambda^*)$ and G denote $\nabla h(x^*)$. Consider the compact set

(4.7) $$S = \{\eta \in R^n : \|\eta\| = 1\} .$$

If the ~~theorem~~ Result is not true, then there exists a sequence $\{\eta_k\}$ in S such that

(4.8) $$\eta_k^T (A + kGG^T)\eta_k \leq \frac{1}{k} , \quad k = 1,2,\ldots \, .$$

But $\{\eta_k\}$ has a convergent subsequence converging to $\bar{\eta} \in S$. Since $\eta^T GG^T \eta \geq 0 \;\; \forall \; \eta$ it follows that

(4.9) $$\bar{\eta}^T GG^T \bar{\eta} = 0 \quad \text{and} \quad \bar{\eta}^T A \bar{\eta} \leq 0 \, .$$

The first part of (4.9) implies that $G^T\bar{\eta} = 0$. The second order necessary conditions, Theorem 1.2, imply that $\bar{\eta}^T A \bar{\eta} \geq 0$, which together with the second part of (4.9) implies that

(4.10) $$\bar{\eta}^T A \bar{\eta} = 0 \, .$$

It follows that the problem

(4.11) $$\text{minimize } \{\tfrac{1}{2}\eta^T A \eta : G^T \eta = 0\}$$

has a solution at $\bar{\eta}$. Hence there exists a multiplier $\mu \in R^m$ such that

$$A\bar{\eta} + G\mu = 0, \quad G^T\bar{\eta} = 0 \, .$$

This implies that the columns of $\nabla^2 \ell(x^*,\lambda^*)$ (see (3.14)) are linearly ~~in~~dependent and contradicts assumption (3.17) . ■

The main problems with this theorem are that it does not tell us what C^* is and it only gives us convexity near the solution.

For the sake of motivation, consider the constrained optimization problem

$$(4.12) \qquad \text{minimize } f(x); \text{ subject to } \ x \in S$$

where S is some subset of R^n. Let

$$(4.13) \qquad \overset{C}{\cancel{\phi}}(x) = \begin{cases} 0 & \text{if } \ x \in S \\ +\infty & \text{if } \ x \notin S \ . \end{cases}$$

Then it is clear that formally the constrained optimization problem (4.12) is equivalent to the unconstrained optimization problem

$$(4.14) \qquad \text{minimize } f(x) + C(x) \ .$$

Clearly problem (4.14) is not acceptable so we must approximate it by problems which are numerically tractable. One way to do this would be to make the approximation

$$(4.15) \qquad Ch(x)^T h(x) \approx C(x)$$

or equivalently

$$(4.16) \qquad P(x;C) \approx f(x) + \overset{c\,h(x)^T h(x)}{\cancel{C(x)}}$$

where C is some positive constant. In fact, the larger C is the better the approximation will be. These ideas lead us to what many refer to as the philosophy of <u>sequential unconstrained minimization techniques</u> or <u>SUMT</u>. Namely, we approximate a solution of problem (EQ) by solving a sequence of unconstrained minimization problems. In the penalty function method the sequence of problems will consist of successive minimizations of the penalty functional $P(x;C)$ with increasing penalty constants.

<u>Exterior Penalty Function Method for Problem (EQ)</u>.

Construct $\{x^k\}$ by solving the sequence of unconstrained minimization problems

$$(4.17) \qquad \min_x P(x;C^k)$$

for some sequence of positive penalty constants C^k, $k = 0,1,2,\ldots$ increasing monotonically to $+\infty$.

Proposition 4.1. Suppose that the exterior penalty function method for problem (EQ) is well defined (i.e., problem (4.10) has a global solution) . Then

(i) $P(x^{k+1};C^{k+1}) \geq P(x^k;C^k)$

(ii) $\|h(x^k)\|_2 \geq \|h(x^{k+1})\|_2$

(iii) $f(x^{k+1}) \geq f(x^k)$

Proof of (i). From (4.17) and the monotonicity of $\{C^k\}$ we have

$$(4.18) \qquad P(x^{k+1};C^{k+1}) \geq P(x^{k+1};C^k) \geq P(x^k;C^k) \ .$$

Proof of (ii). From (4.18) we have

$$(4.19) \qquad P(x^k;C^k) \leq P(x^{k+1};C^k)$$

By the definition of (4.17) we have

$$(4.20) \qquad P(x^{k+1};C^{k+1}) \leq P(x^k;C^{k+1}) \ .$$

Adding (4.19) and (4.20) gives

$$(4.21) \qquad (C^k - C^{k+1})[h(x^k)^T h(x^k) - h(x^{k+1})^T h(x^{k+1})] \leq 0 \ .$$

However, $C^k \leq C^{k+1}$ so (4.21) implies (ii) .

Proof of (iii). From (4.18)

$$(4.22) \qquad f(x^{k+1}) - f(x^k) \geq C^k[h(x^k)^T h(x^k) - h(x^{k+1})^T h(x^{k+1})] \geq 0 \ .$$

This proves (iii) and the proposition. ∎

Proposition 4.2. Suppose that the exterior penalty function method is well defined and converges to a solution of problem (EQ). Then each iterate is necessarily infeasible or is a solution of problem (EQ).

Proof. Suppose $x^k \to x^*$ and x^* solves problem (EQ). By proposition (4.1) we know that $f(x^k) \uparrow f(x^*)$. Therefore, if x^k is feasible, it is a solution. ■

From (4.19) we must have

(4.23) $$\nabla P(x^k;C^k) = \nabla f(x^k) + \nabla h(x^k)C^k h(x^k) = 0 \ .$$

Considering the first order necessary conditions (Theorem 1.1) we are led to the conclusion that $C^k h(x^k)$ is an approximation to the Lagrange multiplier λ^* associated with x^*. Moreover, if $x^k \to x^*$, then $C^k h(x^k) \to \lambda^*$; but $h(x^k) \to 0$, so necessarily $C^k \to +\infty$.

The following main convergence result for the exterior penalty function method is due to Polyak (1971).

(local cond)

Theorem 4.2. Suppose that x^* is a local solution of problem (EQ) and that the standard conditions (3.16) and (3.17) hold. Then there exists a constant $\hat{C} > 0$ such that for every $C > \hat{C}$ the penalty function $P(x;C)$ has a locally unique minimizer, say $x(C)$.

Furthermore, there exists a constant $M > 0$ such that

(4.24) $$\|x(C) - x^*\|_2 \leq M/C \quad \forall\ C > \hat{C}$$

and

(4.25) $$\|Ch(x(C)) - \lambda^*\|_2 \leq M/C \quad \forall\ C > \hat{C} \ .$$

Proof. For a proof see Polak (1971) or Bertsekas (1976). Bertsekas' proof is slightly more general and his conditions are implied by our assumptions.

Corollary 4.1. Suppose that the initial penalty constant in the exterior penalty function method is larger than $\hat{C}$ in Theorem 4.2. Then the exterior penalty function method is convergent if and only if $C \to +\infty$.

Observe that the penalty function method is not really an iterative procedure. Namely, x^{k+1} does not depend on x^k unless the choice of C^{k+1} depends on x^k. The penalty constant C actually plays a role analogous to the role the mesh spacing plays in the solution of differential equations by finite differences. Specifically, we can get arbitrarily good accuracy by choosing the initial penalty constant sufficiently large. The question that should be asked is: Why minimize $P(x;C)$ for various values of C ? Obviously, we need only minimize $P(x;C)$ for the largest value of C that we are interested in. Of course, the numerical conditioning of the problem enters in (as it does in finite differences) and it is not clear what the optimal value of C should be. Our point here is that the nature of the penalty function method is significantly different than that of a standard iterative procedure and is similar, from a philosophical point of view, to the discretization methods in differential equations.
— TALK ABOUT DISCRETIZATION.

The exterior penalty function method can be extended from problem (EQ) to problem (NLP). One merely replaces each inequality constraint $g_i(x) \geq 0$ with the equivalent equality constraint

$$\min(0,g_i(x))=0 \tag{4.26}$$

Not all of our analysis goes through when one works with (4.26) due to the loss of differentiability. However, since $[\min(0,g_i(x))]^2$ is reasonably smooth, much of the analysis presented does carry over to the exterior penalty function for the full problem. In particular, the following simple example will demonstrate Proposition 4.2.

Example 4.1. Consider $\min f(x)$; subject to $x \geq 1$.

We let

$$P(x;C) = x^2 + C \min(0,x-1)^2 .$$

It follows that $x^k = C^k/(1+C^k)$ converges to the solution as $C^k \to +\infty$. However, x^k is always less than one and never feasible.

Consider the special case of problem (NLP) when we only have inequality constraints.

$$\text{minimize } f(x); \quad \text{subject to} \quad g_i(x) \geq 0, \quad i=1,\ldots,m \,. \tag{4.27}$$

We refer to problem (4.27) as problem (INEQ). Consider the function $q: R^n \to R$ given by any one of the following choices

$$q(x) = -\sum_{i=1}^{m} \log(g_i(x)) \tag{4.28}$$

BARRIER FUNCTIONS

$$q(x) = \sum_{i=1}^{m} 1/g_i(x) \tag{4.29}$$

$$q(x) = \sum_{i=1}^{m} 1/g_i(x)^2 \tag{4.30}$$

$$q(x) = \sum_{i=1}^{m} 1/\max(0,g_i(x)) \tag{4.31}$$

Let

$$Q(x;C) = f(x) + \frac{1}{C}q(x) \tag{4.32}$$

<u>Interior Penalty or Barrier Function Method for Problem (INEQ)</u>.

Construct $\{x^k\}$ by solving the sequence of unconstrained minimization problems

$$\min_{x} Q(x;C^k) \tag{4.33}$$

for some sequence of positive penalty C^k, $k=0,1,2,\ldots$, increasing monotonically to $+\infty$. Let $S = \{x: g_i(x) \geq 0, \ i = 1,\ldots,m\}$. Observe that any q given by (4.28) - (4.31) will have the property that $q(x) = +\infty$ when x is contained on the boundary of S (i.e., for some i such that $g_i(x) = 0$). Moreover, $q(x)$ is well defined in the interior of S . It follows that implicit in the optimization problem (4.33) is the assumption that any algorithm used to solve the problem begins in the interior of S and never crosses over the boundary of S into the exterior of S . This is a mild and reasonable requirement since $Q(x;C^k) = +\infty$ on the boundary of S. It follows then that the interior penalty function method always maintains feasibility. This is an important attribute of the approach and one that makes it useful in situations where other approaches cannot be used. Let us demonstrate this aspect of the method with a simple example.

Example 4.2. Consider $\min \frac{1}{2}x$; subject to $x \geq 1$.

We let

$$P(x;C) = \tfrac{1}{2}x + \frac{1}{C}\frac{1}{x-1} .$$

It follows that $x^k = 1 + 2/C^k$ converges to the solution $x^* = 1$ and x^k is always feasible.

In addition to exterior penalty function methods for the full problem, one can also consider mixed penalty function methods where the equality constraints and some of the inequality constraints are handled using the exterior philosophy and the remaining inequality constraints are handled by the certainty interior philosophy.

We leave this section on classical penalty function methods with the following three criticizms of the method.

(i) A sequence of unconstrained minimization problems must be solved leading to questionable efficiency;

(ii) the penalty constants must necessarily become arbitrarily large leading to questionable numerical conditioning;

(iii) it is not clear how the penalty constants should be chosen.

5. Exact Penalty Function Methods. In the penalty function methods presented in Section 4, the solution was obtained by solving a sequence of unconstrained minimization problems. The importance of efficiency leads us to consider the obvious extension of this approach; namely, construct a function with the property that a local minimizer solves the constrained minimization problem.

Definition 5.1. Suppose that $P:R^n \rightarrow R$ has the property that at least one of its local minimizers is a local solution of problem (NLP). Then P is called an exact penalty function for problem (NLP), (see (1.1)).

Zangwill (1967) was one of the first authors to consider exact penalty functions. For problem (INEQ) (see (4.27)) he considered the penalty function

$$P(x;C) = f(x) - C \sum_{i=1}^{m} \min(0, g_i(x)) \tag{5.1}$$

and was able to establish that in special cases $P(x;C)$ was an exact penalty function.

Theorem 5.1. Suppose problem (INEQ) $\in C^1$, f is convex, g_i is concave, $i = 1,\ldots,m$, $S = \{x: g_i(x) > 0,\ i = 1,\ldots,m\} \neq \emptyset$, and x^* is a solution of problem (INEQ). Then there exists $\hat{C} > 0$ such that for all $C \geq \hat{C}$ $P(x;C)$ has x^* as its minimizer.

Proof. A proof can be found in Section 12.4 of Avriel (1976).

Pietrzykowski (1969) extended Zangwill's result to nonconvex programs. Let us consider a simple example.

Example 5.1. Consider $\min x^2$; subject to $x \geq 1$. We let

$$P(x;C) = x^2 - C \min(0, x-1)\ . \tag{5.2}$$

The solution to our constrained optimization problem is $x^* = 1$ and a straightforward calculation will show that $x^* = 1$ minimizes $P(x;C)$ as given by (5.2) as long as $C \geq 2$. This calculation will also show that $P(x;C)$ is not differentiable at $x = 1$. Clearly the Zangwill-Pietrzykowski exact penalty function method has the following two drawbacks

(i) the penalty function is not differentiable at the solution; hence, the more efficient algorithms for unconstrained optimization cannot be used;

(ii) it is not clear how the penalty constant should be chosen.

Fletcher (1970) offered the following approach for constructing an exact penalty function for problem (EQ) (see (3.12)). Let

(5.3) $$\lambda(x) = (\nabla h(x)^T \nabla h(x))^{-1}(\cancel{h(x)} - \nabla h(x)^T \nabla f(x))$$

and consider

(5.4) $$P(x;C) = f(x) + h(x)^T \lambda(x) \;.\quad = L(x, \lambda(x), \rho)$$

Theorem 5.2. Suppose that x^* is a local solution of problem (EQ) and the standard conditions (3.16) and (3.17) hold. Then there exists $\hat{C} > 0$ such that for all $C \geq \hat{C}$ x^* is a local minimizer of $P(x;C)$ given by (5.4).

Proof. For a proof see Fletcher (1970).

The Fletcher exact penalty function method has the following two drawbacks

(i) the penalty function involves first order terms; hence its gradient will involve second order terms and its Hessian will involve third order terms;

(ii) it is not clear how the penalty constant should be chosen .

Recently there has been renewed interest in exact penalty function methods. However, these newer functionals have a slightly different flavor.

Definition 5.2. Consider $P:R^{n+p} \to R$. If P has the property that one of its local minimizers, say (x^*,λ^*) is such that x^* is a local solution to problem (EQ) with associated multiplier λ^*, then we say that P is an exact extended penalty function for problem (EQ) .

The obvious attempt at constructing an extended penalty function is to try the Lagrangian ℓ or the augmented Lagrangian L . While both these functions have the property that they have stationary points which correspond to local solutions and their associated multipliers of problem (EQ); they cannot have local minimizers. To see that neither ℓ nor L can have a local minimizer as functions of (x,λ) merely observe that they are both linear in the variable λ .

Boggs and Tolle (1977) and Boggs, Tolle and Wang (1979), and independently, DiPillo and Grippo (1979) consider the functional

$$(5.5) \qquad P(x,\lambda;C;D) = \ell(x,\lambda) + \frac{C}{2}\, h(x)^T h(x) + \frac{D}{2}\nabla_x \ell(x,\lambda)^T Q(x)\nabla_x \ell(x,\lambda)$$

where D and C are scalars and Q(x) is some weighting matrix function. It should be clear that (5.5) consists of taking the augmented Lagrangian and adding a term which is quadratic in the multiplier λ . In this way there is a good chance that P will have minimizers in (x,λ) . In fact, DiPillo and Grippo (1979) give general conditions which guarantee that P in (5.5) is an exact extended penalty function.

The exact extended penalty function method based on (5.5) suffers from several drawbacks including

(i) the penalty function involves first order terms; hence, its gradient will involve second order terms and its Hessian will involve third order terms.

(ii) it is not clear how the penalty constants C and D should be chosen;

(iii) the dimension of the optimization problem is extended to $n+p$ instead of just n.

6. The Multiplier Method and Nonlinear Duality.

The multiplier method was originally proposed by Hestenes (1969) and independently in different but equivalent forms by Powell (1969) and Haarhoff and Buys (1970). The rationale for the multiplier method is to give a method which is as effective as the penalty function method but does not suffer from the numerical ill-conditioning of the penalty function method, i.e., the penalty constant need not become infinite.

Definition 6.1. A function $U:R^{n+p} \rightarrow R^p$ (which may depend on a parameter C) with the property that

$$\lambda^* = U(x^*,\lambda^*;C)$$

whenever (x^*,λ^*) is a critical point of problem (EQ), is said to be a Lagrange multiplier update formula. Moreover, if U does not depend explicitly on λ, i.e.,

$$\nabla_\lambda U(x,\lambda,C) \equiv 0,$$

then U is said to be a Lagrange multiplier approximation formula.

The multiplier method consists of the iterative procedure: Given λ and $C>0$

(6.1) $$\text{calculate } \bar{x} = \arg\min_x L(x,\lambda;C)$$

(6.2) $$\text{Let } \bar{\lambda} = U(\bar{x},\lambda;C)$$

(6.3) $$\text{Choose } \bar{C}>0$$

where the augmented Lagrangian $L(x,\lambda;C)$ is given by (4.2) and U is a multiplier update formula.

Consider the following choices for the multiplier update formula:

(6.4) $$U_{HP}(x,\lambda;C) = \lambda + Ch(x) ,$$

(6.5) $$U_P(x,\lambda;C) = -[\nabla h(x)^T \nabla h(x)]^{-1} \nabla h(x)^T \nabla f(x) ,$$

(6.6) $$U_B(x,\lambda;C) = \lambda + [\nabla h(x)^T H \nabla h(x)]^{-1} h(x) ,$$

(6.7) $$U_*(x,\lambda;C) = [\nabla h(x)^T H \nabla h(x)]^{-1} [h(x) - \nabla h(x)^T H(\nabla f(x) + C\nabla h(x)h(x))] ,$$

where

$$H = \nabla^2 L(x,\lambda;C)^{-1} ,$$

and more generally

(6.8) $$U_{GUF}(x,\lambda;C) = \lambda + [\nabla h(x)^T D \nabla h(x) + A]^{-1} [h(x) - \nabla h(x)^T D \nabla_x L(x,\lambda;C)]$$

where in (6.8) A and D are $p \times p$ and $n \times n$ matrices respectively, which may depend on x, λ, and C .

Proposition 6.1. The update formulas given by (6.4) - (6.8) are Lagrange multiplier update formulas. Moreover, (6.5) is a Lagrange multiplier approximation formula.

Proof. The proof is straightforward.

The multiplier method using the multiplier update formula (6.4) was proposed independently by Hestenes (1969) and Powell (1969). In 1970, independently of the previous two references, Haarhoff and Buys (1970) proposed the multiplier method using the multiplier update formula (6.5). Observe that the formula (6.5) arises from the least-squares solution for λ of the overdetermined linear system $\nabla_x \ell(x,\lambda) = 0$. The multiplier update formulas (6.5) and (6.6) have been used by many authors in the literature. The formula (6.6) was first used by Buys (1972).

Proposition 6.2. The multiplier update formulas (6.4) - (6.7) are special cases of the multiplier update formula (6.8). Specifically,

(i) $U_{HP} = U_{GUF}$, with $A = (1/C)I$ and $D = 0$;

(ii) $U_P = U_{GUF}$, with $A = 0$ and

$D = (1/C)\nabla g(x)(\nabla g(x)^T \nabla g(x))^{-2} \nabla g(x)^T$;

(iii) $U_B = U_{GUF}$, with $A = \nabla g(x)^T \nabla_x^2 L(x,\lambda;C)^{-1} \nabla g(x)$ and $D = 0$;

(iv) $U_* = U_{GUF}$, with $A = 0$ and $D = \nabla_x^2 L(x,\lambda;C)^{-1}$

Proof. Merely substitute the above choices for A and D in (6.8).

This proposition implies that the update formulas (6.4) - (6.7) are significantly different. We will now show that, in the multiplier method, due to exact minimization, many differences in multiplier update formulas are purely formal.

Proposition 6.3. If the multiplier method is used in conjunction with the update formula U_{GUF}, then no generality is lost by using only formulas with $A = 0$ or only formulas with $D = 0$.

Proof. Let $\hat{D}$ and $\hat{A}$ be arbitrary $n \times n$ and $p \times p$ matrices, respectively. By substituting

$$\nabla_x L(x,\lambda;C) = 0, \qquad A = 0,$$

and

$$D = \hat{D} + \nabla h(x)(\nabla h(x)^T \nabla h(x))^{-1} \hat{A} (\nabla h(x)^T \nabla h(x))^{-1} \nabla h(x)^T$$

into (6.8), we see that no generality has been lost by letting $A = 0$. The corresponding statement for D is obvious. ∎

Proposition 6.4. In the multiplier method the multiplier update formulas U_{HP} and U_P give identical iterates as do the multiplier update formulas U_B and U_* .

Proof. The proof follows directly from the fact that exact minimization implies $\nabla_x L(x,\lambda;C) = 0$. ■

It is of historical interest to observe that, as a consequence of Proposition 6.4, we have that, even though Haarhoff and Buys used a different multiplier update formula, their multiplier method is equivalent (gives the same iterates) to the Hestenes-Powell multiplier method.

We first analyze the role of the multiplier update formula (6.4) and the specific role of the penalty constant in this formula. This will be accomplished by looking at the nonlinear duality theory. Let x^* be the nonsingular solution of problem (EQ) with associated Lagrange multiplier λ^* . Assume that $C > C^*$ where C^* is given in Theorem 4.1 . By the implicit function theorem (p. 128 of Ortega and Rheinboldt (1970)), there exists a neighborhood W of λ^* and a function $x: W \subset R^m \to R^n$, with the following properties:

(6.9) $$x(\lambda^*) = x^* ,$$

(6.10) $$\nabla_x L(x(\lambda),\lambda;C) = 0$$

(6.11) $$\nabla x(\lambda) = -\nabla h(x(\lambda))^T \nabla_x^2 L(x(\lambda),\lambda;C)^{-1} ,$$

and

(6.12) $$\Phi(\lambda) = \min_x L(x,\lambda;C)$$

is well defined on W . Problem (EQ) (see(3.12)) is called the primal problem . The dual problem is defined below:

(6.13) $$\max_\lambda \Phi(\lambda) .$$

OR $\max_\lambda L(x,\lambda;C)$ s.t. $\nabla_x L(x,\lambda;C) = 0$

In (6.13) we have tacitly assumed that λ is restricted to the open set W. Since

$$\Phi(\lambda) = L(x(\lambda),\lambda;C) \tag{6.14}$$

using (6.10) and (6.11) we see that

$$\nabla\Phi(\lambda) = h(x(\lambda)) , \tag{6.15}$$

$$\nabla^2\Phi(\lambda) = -\nabla h(x(\lambda))^T \nabla_x^2 L(x(\lambda),\lambda;C)^{-1} \nabla h(x(\lambda)) . \tag{6.16}$$

From Theorem 4.1, $\nabla_x^2 L(x^*,\lambda^*;C)$ is positive definite; so $\nabla^2\Phi(\lambda^*)$ is negative definite. Combining these remarks leads us to the following duality principle:

<u>Theorem 6.1</u>. (Local Duality). If x^* solves the primal problem, then its associated Lagrange multiplier λ^* solves the dual problem and x^* can be obtained from λ^* as the solution of $\min_x L(x,\lambda^*;C)$.

As a consequence of local duality we have the following characterization of the multiplier method.

<u>Theorem 6.2</u>. The class of algorithms for the primal problem given by the multiplier method with a multiplier update formula of the form (6.8) is exactly the class of quasi-Newton methods for the dual problem. In particular, the multiplier method with multiplier update formula (6.4) or (6.5) is the gradient method (with fixed steplength) applied to the dual problem; and the multiplier method with multiplier update formula (6.6) or (6.7) is Newton's method applied to the dual problem.

From Proposition 6.3, we see that the above proposition would still be true if we only considered multiplier update formulas of the form (6.8), with $A = 0$ or, equivalently, $D = 0$.

Consider the multiplier method as given by (6.1) - (6.3). One function that the penalty constant has is to make step (6.1) well defined as dictated by Theorem 4.1. Another role that it plays, according to (6.2) and Theorem 6.1, is that of acting as the step length in the gradient method applied to the dual problem. This latter role tells us from gradient method theory we will be able to obtain local linear convergence for a range of penalty constants. This range will depend on the eigenvalue structure of the Hessian matrix $\nabla_x^2 L(x^*,\lambda^*;C)$. Moreover, we are led to believe that, in contrast to the penalty function method, we cannot let the penalty constant grow arbitrarily fast. In fact, at this point we do not even know if it is possible to let the penalty constant become infinite and if anything would be gained by such a choice.

We now consider local convergence and convergence rates for the multiplier method. Bertsekas (1976) generalized Polyak's theorem (Theorem 4.2) to include the multiplier method in the following manner. As before, we are assuming the standard conditions (3.16) and (3.17) and x^* is a local solution of problem (EQ) with associated multiplier λ^*.

Theorem 6.3. Let S be a bounded subset of R^p which contains λ^* as an interior point. Then there exists a constant $\hat{C}$ such that for $C > \hat{C}$ and $\lambda \in S$ the augmented Lagrangian $L(x,\lambda;C)$ has a locally unique minimizer, say $x(\lambda;C)$. Furthermore, there exists a constant $M > 0$ such that

(6.17) $$\|x^* - x(\lambda;C)\|_2 \le \frac{M}{C}\|\lambda - \lambda^*\| ,$$

and

(6.18) $$\|\lambda^* - \bar{\lambda}(\lambda;C)\|_2 \le \frac{M}{C}\|\lambda - \lambda^*\| , \quad \forall\ C > \hat{C} \text{ and } \forall\ \lambda \in S$$

where

(6.19) $$\bar{\lambda}(\lambda;C) = \lambda + Cg(x(\lambda;C)) .$$

Several questions immediately come to mind concerning local convergence and convergence rates of the multiplier method and we shall attempt to answer these questions in the remainder of this section. To begin with, from (6.18) of Theorem 6.3, we expect to be able to analyze convergence of λ in terms of Q-convergence. However, (6.17) does not lead to the same conjecture in terms of the convergence of x. In fact, on the surface it looks as if one might have to settle for an analysis in terms of R-convergence. For definitions of these convergence notions see Section 8 of Tapia (1977) and for more detail see Chapter 9 of Ortega and Rheinboldt (1970). The following result proved in Section 9 of Tapia (1977) gives us the satisfaction that the convergence in x and λ is essentially the same.

Proposition 6.4. Suppose that the multiplier method with an arbitrary Lagrange multiplier update formula and an arbitrary bounded sequence of penalty constants $\{C^k\}$ such that $C^k \geq \hat{C}$ generates the sequences $\{x^k\}$ and $\{\lambda^k\}$. Then $\lambda^k \to \lambda^*$ with Q-order q if and only if $x^k \to x^*$ with Q-order q.

Proof. The proof of this result is given in Section 9 of Tapia (1977).

As a direct consequence of Theorem 6.3 and Proposition 6.4 we have the following convergence result for the multiplier method.

Proposition 6.5. For any given initial estimate of the Lagrange multiplier λ there exists a penalty constant $\hat{C} > 0$ such that the multiplier method with fixed penalty constant $C > \hat{C}$ is Q-linearly convergent in x and in λ.

Observe that in the multiplier method the penalty constant cannot be increased arbitrarily fast as it can in the penalty function method. If it grows too fast, then $\bar{\lambda}(\lambda;C)$ given by (6.19) will become excessively large (i.e., it will not remain in the set S in Theorem 6.3) and the convergence will suffer. It is clear that the increase in C must be balanced with the decrease in $h(x)$. However, from (6.18) we see that Q-superlinear convergence would result if it were possible to let the sequence of penalty constants become unbounded. This latter consideration is the subject of the following proposition.

Proposition 6.6. It is possible to choose $\{C^k\}$ so that $C^k \to \infty$ and the multiplier method with penalty constant $\{C^k\}$ is convergent in x and λ.

Proof. The proof follows directly from Theorem 6.3. Specifically, let $S = \{\lambda : ||\lambda - \lambda^*|| \le 1\}$, and choose $C^0 > \hat{C}$ so that $M/C^0 < \frac{1}{2}$ and choose λ^0 so that $||\lambda^* - \lambda^0|| < \frac{1}{2}$. Then

$$(6.20) \qquad ||x^* - x^k|| \le \frac{1}{2^k} \quad \text{and} \quad ||\lambda^* - \lambda^k|| \le \frac{1}{2^k}$$

as long as $C^k \ge C^0$ and

$$(6.21) \qquad C^k ||g(x^k)|| \le \tfrac{1}{2} .$$

From (6.21) it is clear that we can choose $\{C^k\}$ so that $C^k \to \infty$. ■

We are concerned with the role of the penalty constant in the multiplier method. So far we have seen that it allows one to obtain Q-linear convergence and Q-superlinear convergence if it becomes infinite. Recall that in the penalty function method we obtained convergence if and only if the penalty constant became infinite. The situation would be mathematically satisfying if the analogous situation for the multiplier method was such that we were able to obtain superlinear convergence if and only if the penalty constant became infinite. The following proposition establishes this fact. For the purposes of this result we will assume that $\hat{C} = 0$.

Proposition 6.7. Suppose that the multiplier method with penalty constants C^k is convergent. Then the convergence is Q-superlinear in λ if and only if $C^K \to \infty$.

Proof. The 'if' part follows directly from Theorem 6.3. Assume that λ^k converges Q-superlinearly to λ^*. We are concerned with the iteration

(6.22) $$\lambda^{k+1} = S(\lambda^k;C^k)$$

where

(6.23) $$S(\lambda;C) = \lambda + Cg(x(\lambda))$$

and $x(\lambda)$ is as in (6.9) - (6.16). Now for a fixed C we see from (6.11) that

(6.24) $$S'_\lambda(\lambda^*;C) = I - C\nabla g(x^*)^T \nabla_x^2 L(x^*,\lambda^*;C)^{-1} \nabla g(x^*) .$$

Let $A = \nabla_x^2 \ell(x^*,\lambda^*)$ and $G = \nabla h(x^*)$ so that

(6.25) $$\nabla_x^2 L(x^*,\lambda^*) = A + CGG^T$$

and from (6.24)

(6.26) $$S'_\lambda(\lambda^*;C) = I - CG^T(A + CGG^T)^{-1}G .$$

From the Sherman-Morrison-Woodbury formula (page 50 of Ortega and Rheinboldt (1970)) we obtain

(6.27) $$(A + CGG)^T)^{-1} = A^{-1} + CA^{-1}G(I + CG^TA^{-1}G)^{-1}G^TA^{-1} .$$

so that

(6.28) $$S'_\lambda(\lambda^*;C) = [I + C\nabla g(x^*)^T \nabla_x^2 \ell(x^*,\lambda^*)^{-1} \nabla g(x^*)]^{-1} .$$

Observe that for $C \geq 0$ the matrix $S'_\lambda(\lambda^*;C)$ is positive definite and hence invertible.

From McLeods's mean-value theorem (see Tapia (1971)) we have

(6.29) $$\lambda^{k+1} - \lambda^* = S(\lambda^k;C^k) - \lambda^* = \sum_{i=1}^m t_i S'_\lambda(\lambda^* + \theta_i(\lambda^k - \lambda^*);C^k)(\lambda^k - \lambda^*$$

where

$$0 < \theta_i < 1, \quad t_i \geq 0, \quad \sum_{i=1}^m t_i = 1 .$$

Suppose that a subsequence of $\{C^k\}$ (also denoted by $\{C^k\}$) converges to $K<+\infty$. Let

(6.30) $$s_k = (\lambda^k - \lambda^*)\|\lambda^k - \lambda^*\|^{-1} .$$

By compactness, $\{s_k\}$ has a subsequence (which we also denote by $\{s_k\}$) which converges to $s^* \neq 0$. Dividing both sides of (6.22) by $\|\lambda^k - \lambda^*\|$, we obtain

(6.31) $$S'_\lambda(\lambda^*;K)(s^*) = 0 .$$

However, this is a contradiction, since $S'_\lambda(\lambda^*;K)$ is invertible. It follows that $C^k \to \infty$ and this proves the proposition. ■

Our analysis of the role of the penalty constant in the multiplier method is now complete.

7. The Diagonalized Multiplier Method. Let us summarize our presentation up to this point from a historical and chronological point of view. We have observed that in the penalty function method the price one pays for convergence is a deterioration in numerical conditioning, since the penalty constant must go to infinity. In the multiplier method, the price one pays for superlinear convergence is also a deterioration in numerical conditioning, since again the penalty function must go to infinity. Clearly, the stage was set to a multiplier-like algorithm which would give superlinear convergence without a corresponding deterioration in numerical conditioning. Such an algorithm will now be presented.

Historically, there have been essentially three philosophies for extending quasi-Newton methods from unconstrained optimization to constrained optimization. These philosophies consist of the extended problem approach described in Section 3, the diagonalized multiplier method which we are about to describe and the successive quadratic programming approach described in the following section .

By using a multiplier method on problem (EQ), we are in effect trying to solve for both the minimizer x^* and its associated Lagrange multiplier λ^*. Hence, it makes sense to update the estimate of the multiplier after each update of the estimate of the minimizer and so make the two update formulas compatible, i.e., they both use first-order information only, or they both use second-order information, etc.

The Diagonalized Multipler Method consists of the iterative procedure: Given x, λ, B and C

$$\bar{\lambda} = U(x,\lambda;C) \tag{7.1}$$

$$\bar{x} = x - B^{-1}\nabla_x L(x,\bar{\lambda};C) \tag{7.2}$$

$$\bar{B} = \mathcal{B}(x,\bar{x},\lambda,\bar{\lambda},B) \tag{7.3}$$

where U is a multiplier update formula and $\mathcal{B}(x,\bar{x},\lambda,\bar{\lambda},B)$ is an approximation to $\nabla_x^2 L(\bar{x},\bar{\lambda};C)$. The diagonalized multiplier secant methods result by choosing

$$\mathcal{B}(x,\bar{x},\lambda,\bar{\lambda},B) = \mathcal{B}_S(s,y,B) \tag{7.4}$$

where $s = \bar{x} - x$, $y = \nabla_x L(\bar{x},\bar{\lambda};C) - \nabla_x L(x,\bar{\lambda};C)$ and $\mathcal{B}_S$ is a secant update formula, e.g., the BFGS (see Section 3).

In the diagonalized multiplier method with U_B (see 6.6)), or U_* (see 6.7)) we choose H to be B^{-1} and not $\nabla_x^2 L(\bar{x},\bar{\lambda};C)^{-1}$. We also want to work with the extended problem using the augmented Lagrangian $L(x,\lambda;C)$ instead of the classical Lagrangian $\ell(x,\lambda)$. To denote this we will say the extended problem with L for problem (EQ).

Consider the following class of quasi-Newton methods for the extended problem with L for problem (EQ).

$$(7.5) \qquad \begin{bmatrix} B & \nabla h(x) \\ \overset{\nabla h^T DB}{\cancel{S}} & \overset{-A}{\cancel{T}} \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta\lambda \end{bmatrix} = - \begin{bmatrix} \nabla_x L(x,\lambda;C) \\ h(x) \end{bmatrix}$$

where B^{-1} and $[SB^{-1}\nabla h(x) - T]^{-1}$ exist .
$[\nabla h' D \nabla h + A]^{-1}$

Theorem 7.1. The class of algorithms for problem (EQ) given by the diagonalized multiplier method with U_{GUF} (see (6.8)) is exactly the class of quasi-Newton methods of the form (7.5) for the extended problem with L . In particular, using U_* (see 6.7)) the diagonalized Newton multiplier method is equivalent to Newton's method on the extended problem with L . Finally, using U_* a diagonalized secant multiplier method is equivalent to a structured secant method for the extended problem with L .

Proof. If we write out the two equations in (7.5), and solve the first for Δx and then substitute Δx into the second, we obtain

$$(7.6) \qquad \Delta\lambda = [SB^{-1}\nabla h(x) - T]^{-1}[h(x) - SB^{-1}\nabla_x L(x,\lambda;C)] \ .$$

From (7.6) we see that the association between B, S, and T in (7.5) and A and D in (6.8) is

$$(7.7) \qquad T = -A \quad \text{and} \quad S = \nabla h(x)^T DB \ .$$

Now, from Proposition 6.2 we see that U_* results when $A = 0$ and $D = B^{-1}$, which in turn give $T = 0$ and $S = \nabla h(x)^T$. ∎

It is of interest to also characterize the diagonalized multiplier method using U_{Hp}, U_p and U_B in terms of a quasi-Newton method on the extended problem with L . From (7.7) and Proposition 6.2 we are led to the following characterizations of the diagonalized multiplier method in terms of the extended problem with L :

$\underline{U_{HP}}$:

$$\begin{pmatrix} B & \nabla g \\ 0 & -\frac{1}{c} I \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta\lambda \end{pmatrix} = - \begin{bmatrix} \nabla_x L(x,\lambda;C) \\ h(x) \end{bmatrix}$$

$\underline{U_P}$:

$$\begin{pmatrix} B & \nabla h \\ \frac{1}{C}(\nabla h^T \nabla h)^{-1} \nabla h B & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta\lambda \end{pmatrix} = - \begin{pmatrix} \nabla_x L(x,\lambda;C) \\ h(x) \end{pmatrix}$$

$\underline{U_B}$:

$$\begin{pmatrix} B & \nabla h \\ 0 & -\nabla h^T B^{-1} \nabla h \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta\lambda \end{pmatrix} = - \begin{pmatrix} \nabla_x L(x,\lambda;C) \\ h(x) \end{pmatrix}$$

$\underline{U_*}$:

$$\begin{pmatrix} B & \nabla h \\ \nabla h^T & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta\lambda \end{pmatrix} = - \begin{pmatrix} \nabla_x L(x,\lambda;C) \\ h(x) \end{pmatrix}$$

Theorem 7.1 allows us to give the convergence analysis for the diagonalized secant multiplier method merely as a restatement of Theorem 3.1.

Corollary 7.1. Let x^* be a local solution of problem (EQ). Assume that the standard conditions (3.15) and (3.16) hold and that $C > \hat{C}$ where $\hat{C}$ is given by Theorem 4.1. Then the diagonalized BFGS secant multiplier method using U_* is locally Q-superlinearly convergent in the variable (x,λ) .

In an impressive work, Glad (1979) has established local linear convergence of the diagonalized BFGS secant multiplier method using U_{HP} and U_P .

It is interesting that the logical conclusion of improving the penalty function method led to quasi-Newton algorithms which are essentially the structured quasi-Newton methods for the extended problem.

8. Successive Quadratic Programming. By a successive quadratic programming quasi-Newton method (SQP) for problem (EQ) we mean the iterative procedure:

Given x, λ, B and C

(8.1) $$\bar{x} = x + \Delta x$$

(8.2) $$\bar{B} = \mathcal{B}(x,\bar{x},B)$$

where $\mathcal{B}(x,\bar{x},B)$ is an approximation to $\nabla_x^2 L(x,\lambda;C)$ and Δx is the solution of the quadratic program

(8.3) $$\min q(\Delta x) = \nabla F(x)^T \Delta x + \tfrac{1}{2}\Delta x^T B \Delta x$$

$$\text{subject to} \quad \nabla h(x)^T \Delta x + h(x) = 0$$

with

(8.4) $$F(x) = f(x) + \frac{C}{2} h(x)^T h(x) .$$

The <u>successive quadratic programming secant methods</u> result by choosing $\mathcal{B}(x,\bar{x},B) = \mathcal{B}_S(x,y,B)$ where $s = \bar{x} - x$, $y = \nabla_x L(\bar{x},\lambda_{QP};C) - \nabla_x L(x,\lambda_{QP};C)$, $\mathcal{B}_S$ is a secant update and λ_{QP} is the multiplier obtained in the solution of the quadratic program (8.3). Since B in (6.3) is an approximation to $\nabla_x^2 L(x,\lambda;C)$ it is natural to ask if anything could be gained by replacing the quadratic program (8.3) with the quadratic program

(8.5) $$\min_{\Delta x} q(\Delta x) = \nabla_x L(x,\lambda;C)^T \Delta x + \tfrac{1}{2}\Delta x^T B \Delta x$$

$$\text{subject to} \quad \nabla h(x)^T \Delta x + h(x) = 0 .$$

The following proposition shows that nothing would be gained.

<u>Proposition 8.1</u>. The quadratic programs (8.3) and (8.5) have the same solutions.

<u>Proof</u>. Notice that $L(x,\lambda;C) = F(x) + \lambda^T h(x)$ and so

(8.6) $$\nabla_x L(x,\lambda;C)^T \Delta x = \nabla F(x)^T \Delta x + \lambda^T \nabla h(x)^T \Delta x .$$

However, since we require $\nabla h(x)^T \Delta x = -h(x)$ we see that the second term on the right-hand side of (8.6) does not vary with ~~x~~ Δx. ∎

Given x, λ, B and C

$$\bar{x} = x + \Delta x \tag{8.1}$$

$$\bar{B} = \mathcal{B}(x,\bar{x},B) \tag{8.2}$$

where $\mathcal{B}(x,\bar{x},B)$ is an approximation to $\nabla_x^2 L(x,\lambda;C)$ and Δx is the solution of the quadratic program

$$\min\ q(\Delta x) = \nabla F(x)^T \Delta x + \tfrac{1}{2}\Delta x^T B \Delta x \tag{8.3}$$

$$\text{subject to}\quad \nabla h(x)^T \Delta x + h(x) = 0$$

with

$$F(x) = f(x) + \frac{C}{2}\, h(x)^T h(x)\ . \tag{8.4}$$

The <u>successive quadratic programming secant methods</u> result by choosing $\mathcal{B}(x,\bar{x},B) = \mathcal{B}_S(x,y,B)$ where $s = \bar{x} - x$, $y = \nabla_x L(\bar{x},\lambda_{QP};C) - \nabla_x L(x,\lambda_{QP};C)$, $\mathcal{B}_S$ is a secant update and λ_{QP} is the multiplier obtained in the solution of the quadratic program (8.3). Since B in (6.3) is an approximation to $\nabla_x^2 L(x,\lambda;C)$ it is natural to ask if anything could be gained by replacing the quadratic program (8.3) with the quadratic program

$$\min_{\Delta x}\ q(\Delta x) = \nabla_x L(x,\lambda;C)^T \Delta x + \tfrac{1}{2}\Delta x^T B \Delta x \tag{8.5}$$

$$\text{subject to}\quad \nabla h(x)^T \Delta x + h(x) = 0\ .$$

The following proposition shows that nothing would be gained.

<u>Proposition 8.1</u>. The quadratic programs (8.3) and (8.5) have the same solutions. However the associated mult change $\lambda_F = \lambda + \Delta\lambda_L$

<u>Proof</u>. Notice that

$$\nabla_x L(x,\lambda;C)^T \Delta x = \nabla F(x)^T \Delta x + \lambda^T \nabla h(x)^T \Delta x\ . \tag{8.6}$$

However, since we require $\nabla h(x)^T \Delta x = -h(x)$ we see that the second term on the right-hand side of (8.6) does not vary with ~~λ~~ Δx. ■

Theorem 8.1. For problem (EQ) as given by (3.12), using the matrix update formula $\mathcal{B}$ the following three philosophies generate identical (x,λ) iterates:

(i) the structured quasi-Newton method for the extended problem with L ,

(ii) the diagonalized quasi-Newton method using U_* ,

(iii) the successive quadratic programming quasi-Newton method.

Proof. Problem (8.3) is equivalent to

$$\nabla f(x) + B\Delta x + \nabla h(x)[\lambda_{QP} + Ch(x)] = 0 \tag{8.7}$$

$$\nabla h(x)^T\Delta x + h(x) = 0 \ . \tag{8.8}$$

From (8.7) we see that

$$\Delta x = -B^{-1}\nabla_x L(x,\lambda_{QP};C) \ . \tag{8.9}$$

Substituting (8.9) into (8.8) and solving for λ_{QP} gives $\lambda_{QP} = U_*(x,\lambda;C)$ where U_* is given by (6.7). The proof now follows from Proposition 7.1. ∎

Corollary 8.1. Let x^* be a local solution of problem (EQ). Assume that the standard conditions (3.16) and (3.17) hold and that $C > \hat{C}$ where $\hat{C}$ is given by Theorem 4.1. Then the successive quadratic programming BFGS secant method is locally Q-superlinearly convergent in the variable (x,λ) .

Of the three equivalent formulations the SQP philosophy is by far the most visible and most popular. This is fair since it allows one to use existing quadratic programming modules. The main reason for the popularity of the SQP method is that it allows one to include inequality constraints in a straightforward manner; one merely carries them along as linearized inequalities in the quadratic program. This is a very important consideration.

Mathematically the situation is not well-defined since the theory for handling the inequalities will now be a function of the quadratic programming code employed in the implementation and vary significantly. It is not clear if the quadratic programming formulation offers satisfactory ways of handling the inequalities which could not be employed with one of the equivalent formulations. Further research on this subject is needed.

It is important to emphasize modulo the treatment of inequality constraints the SQP method is no different than our other two approaches. This point is not fully appreciated by all workers in the area.

9. Superstructure and the Penalty Constant. The role of the penalty constant C should now be clear. In the penalty function method it gave us convergence, in the multiplier method it gave us superlinear convergence and in our three equivalent approaches it allowed us to obtain a positive definite Hessian $\nabla_x^2 L(x^*,\lambda^*;C)$. Moreover, the standard BFGS secant theory requires that the Hessian at the solution be positive definite. So everything fits together nicely in the sense that we are approximating a positive definite matrix by a sequence of positive definite matrices. However, the story is not over yet. We now look a little closer at the role of the penalty constant.

Observe that a straightforward quasi-Newton method for the extended problem with L would consist of approximating the entire Hessian matrix

(9.1) $$\nabla^2 L(x,\lambda;C) = \begin{pmatrix} \nabla_x^2 L(x,\lambda;C) & \nabla h(x) \\ \nabla h(x)^T & 0 \end{pmatrix}$$

Our quasi-Newton approach has not been that näive. Specifically, we have taken advantage of a certain amount of structure that the problem has to offer by only approximating the component of $\nabla^2 L(x,\lambda,C)$ in (9.1) which contains second order information. Basically, it seems inefficient to approximate first order information that has already been calculated exactly, or even worse yet, to approximate the zero component in $\nabla^2 L(x,\lambda;C)$. Carrying this line of reasoning one step further we observe that

$$\nabla_x^2 L(x^*,\lambda^*;C) = \nabla_x^2 \ell(x^*,\lambda^*) + C\nabla h(x^*)\nabla h(x^*)^T \ . \tag{9.2}$$

Consequently, although we have taken advantage of some structure, we have more, i.e., we need not approximate the first order information in (9.2). This additional structure we call superstructure. We take advantage of superstructure by replacing $\bar{B}_x$ in the structured secant method for the extended problem (see (3.19)), $\bar{B}$ in the diagonalized multiplier secant method (see (7.3)) and $\bar{B}$ in the successive quadratic programming secant method (see (8.2)).

$$M_S(s,y,M) + C\nabla h(\bar{x})\nabla h(\bar{x})^T \tag{9.3}$$

where

$$s = \bar{x} - x \ , \tag{9.4}$$

$$y = \nabla_x \ell(\bar{x},\bar{\lambda}) - \nabla_x \ell(x,\bar{\lambda}), \tag{9.5}$$

M is the current approximation to $\nabla_x^2 \ell(x,\lambda)$ and M_S is a secant update.

<u>Theorem 9.1</u>. The superstructured versions of the structured secant method for the extended problem with L, the diagonalized secant multiplier method using U_* and the successive quadratic programming secant methods, generate identical (x,λ) iterates which are independent of the penalty constant C.

<u>Proof</u>. The equivalence is the same as before. For the independence of C observe that in the case $B = M + C\nabla h(x)\nabla h(x)^T$ the system (8.7) and (8.8) reduces to the system

$$(9.6) \qquad M\Delta x + \nabla f(x) + \nabla h(x)\lambda_{QP} = 0$$

$$(9.7) \qquad \nabla h(x)^T \Delta z + h(x) = 0 \ .$$

We are assuming that the initial M matrix is independent of C; hence, Δx and λ_{QP} obtained from (9.6) - (9.7) will be independent of C, and from (9.5) we see that $\bar{M}$ will be independent of C. ∎

We can say with some confidence that taking advantage of available structure is worthwhile since it obviously leads to better approximate Hessians. However, acceptance of this statement implies that there is no need for the penalty constant and we have followed the role of the penalty constant to its logical conclusion.

In the literature we have seen several authors argue that the penalty constant should not be used because it is difficult to choose and its use merely makes the algorithm messy. Of course, we have had to accept this denial of the penalty constant in the context that it was made; namely, with little confidence.

Unless we are willing to assume that $\nabla_x^2 \ell(x^*,\lambda^*)$ is positive definite we have no local convergence theory for these secant methods for constrained optimization. Currently there is considerable work being performed in this area.

10. Global Behavior and Step-length Control. The implementation and convergence theory we have presented for the structured quasi-Newton methods for the extended problem and equivalent algorithms has been local. Namely, we will have convergence at the proper rate if both the initial iterate and the initial approximation to the Hessian are close to the solution and the Hessian at the solution respectively. We now consider one approach that can be employed when it is not known whether we are near the solution or not.

We will introduce step-length control in the structured quasi-Newton methods for the extended problem. It will then follow that our comments and ideas can be carried over, in the obvious way, to the equivalent diagonalized quasi-Newton methods and to the equivalent successive quadratic programming quasi-Newton methods.

By step-length control in the structured quasi-Newton method for the extended problem with L we mean the inclusion of α in (3.14) in the following form

$$\begin{pmatrix} \bar{x} \\ \bar{\lambda} \end{pmatrix} = \begin{pmatrix} x \\ \lambda \end{pmatrix} - \alpha B^{-1} \nabla L(x,\lambda;C) \ . \tag{10.1}$$

We know from the Dennis-Moré theory that α must approach 1 if we are to retain superlinear convergence. So, locally the choice $\alpha = 1$ is optimal. However, choosing $\alpha = 1$ when the iterates are far from the solution could be disastrous; one approach is called back tracking. Namely, given a merit function, say, $\Phi(x,\lambda;C)$, try $\alpha = 1$ in (10.1). If satisfactory reduction or behavior is obtained in terms of the merit function, then accept $\alpha = 1$; otherwise, cut α down and re-evaluate the behavior in terms of the merit function (for details see Chapter 5 of Dennis and Schnabel (1981)).

Obvious choices for merit functions when dealing with problem (EQ) as given in (3.12) are the classical ℓ_2-penalty function

$$\Phi(x,\lambda;C) = f(x) + \frac{C}{2} h(x)^T h(x) \ , \tag{10.1}$$

the ℓ_1-penalty function

$$\Phi(x,\lambda;C) = f(x) + C \sum_{i=1}^{p} |h_i(x)| , \tag{10.2}$$

the classical Lagrangian

$$\Phi(x,\lambda;C) = f(x) + \lambda^T h(x) \ , \tag{10.3}$$

the augmented Lagrangian

(10.4) $$\Phi(x,\lambda;C) = f(x) + \lambda^T h(x) + \frac{C}{2} h(x)^T h(x) \ ,$$

the ℓ_2-norm squared of the gradient of the augmented Lagrangian

(10.5) $$\Phi(x,\lambda;C) = \nabla_x L(x,\lambda;C)^T \nabla_x L(x,\lambda;C) + h(x)^T h(x) \ ,$$

the exact penalty function used by Boggs-Tolle-Wang (1979) and DePillo-Grippo (1979)

(10.6) $$\Phi(x,\lambda;C) = f(x) + \lambda^T h(x) + \frac{C}{2} h(x)^T h(x) + \frac{D}{2} \nabla_x \ell(x,\lambda)^T Q(x) \nabla_x \ell(x,\lambda) \ .$$

These merit functions can all be extended to problems with inequality constraints by adding a term of the form $\min(0,g_i(x))$ for each inequality constraint of the form $g_i(x) \geq 0$. In (10.5) and (10.6) one should probably work with $\min(0,g_i(x))^2$.

There are numerous studies in the literature concerned with determining the effectiveness of one of the merit functions given above. A nice global convergence analysis was given by Dixon (1979) for the merit functions (10.5) and (10.6). Biggs uses (10.1) to globalize his version of the SQP algorithm. Han (1977) and Powell (1977) use (10.2). Tapia (1977) suggests the use of (10.5) and Bertocchi, Cavalli and Spedicato (1979) give several numerical examples using (10.5).

REFERENCES

Avriel, M. (1976). Nonlinear Programming: Analysis and Methods, Prentice-Hall, Englewood Cliffs, New Jersey.

Bertocchi, M., Cavalli, E. and Spedicato, E. (1979). Computational Performance of Diagonalized Multiplier Quasi-Newton Methods for Nonlinear Optimization with Equality Constraints, in Numerical Optimization of Dynamic Systems, 1, C. W. Dixon and G. P. Szego (eds.), North Holland, Amsterdam, pp 247-268.

Bertsekas, D. P. (1976). On Penalty and Multiplier Methods for Constrained Minimization, SIAM J. on Control and Optimization, Vol. 14, pp. 216-235.

Biggs, M. D. (1978). On the Convergence of Some Constrained Minimization Algorithms Based on Recursive Quadratic Programming, J. Inst. Math. Applications, Vol. 21, pp. 67-81 .

Boggs, P. T., Tolle, J. W. and Wang, P. (1979). On Quasi-Newton Methods for Constrained Optimization, Report No. 78-8, Operations Research and Systems Analysis, Univ. of North Carolina, Chapel Hill, North Carolina 27514.

Buys, J. D. (1972). Dual Algorithms for Constrained Optimization, Ph.D. Thesis, Rijksuniversiteit de Leiden.

Dennis, J. E. and Moré, J. J. (1977). Quasi-Newton Methods:Motivation and Theory, SIAM Review, Vol. 10, pp. 46-89.

Dennis, J. E. and Schnabel, R. B. (1981). Quasi-Newton Methods for Unconstrained Nonlinear Problems, manuscript in preparation.

DiPillo, G. and Grippo, L. (1979). A new class of Augmented Lagrangians in Nonlinear Programming, SIAM J. Control and Optimization, pp.618-628.

Dixon, L. C. W. (1980). Exact Penalty Function Methods in Nonlinear Programming, in Numerical Optimization of Dynamic Systems, L. C. W. Dixon and G. P. Szego (eds.), North Holland, Amsterdam, pp. 33-54.

Fiacco, A. V. and McCormick, G. P. (1968). Nonlinear Programming: Sequential Unconstrained Minimization Techniques, John Wiley, New York.

Fletcher, R. (1970). A Class of Methods for Nonlinear Programming with Termination and Convergence Properties, in Integer and Nonlinear Programming, J. Abadie (ed.), North Holland, Amsterdam.

Garcia Palomares, U. M. and Mangasarian, O. L. (1976). Superlinearly Convergent Quasi-Newton Algorithms for Nonlinearly Constrained Optimization Problems, Mathematical Programming, Vol. 11, pp. 1-13.

Glad, T. (1979). Properties of Updating Methods for the Multipliers in Augmented Lagrangians, Journal of Optimization Theory and Applications, Vol. 28, pp. 135-156.

Haarhoff, P. C. and Buys, J.D. (1970). A New Method for the Optimization of a Nonlinear Function Subject to Nonlinear Constraints, Computing Journal, Vol. 13, pp. 178-184.

Han, S. P. (1976). Superlinearly Convergent Variable Metric Algorithms for General Nonlinear Programming Problems, Mathematical Programming, Vol. 11, pp. 263-282.

Han, S. P. (1977). Dual Variable Metric Algorithms for Constrained Optimization, SIAM J. on Control and Optimization, Vol. 15, pp. 546-565.

Hestenes, M. R. (1969). Multiplier and Gradient Methods, J. Optimization Theory Appl., Vol. 4, pp. 303-320.

Luenberger, D.G. (1973). Introduction to Linear and Nonlinear Programming, Addison-Wesley, Reading, Mass.

Mangasarian, O. L. (1969). Nonlinear Programming, McGraw-Hill, New York.

Ortega, J. M. and Rheinboldt, W. C. (1970). Iterative Solution of Nonlinear Equations in Several Variables, Academic Press, New York, N New York.

Pietrzykowski, T. (1969). An Exact Potential Method for Constrained Maxima, SIAM J. Numer. Anal., Vol. 6, pp. 299-304.

Polyak, B. T. (1971). The Convergence Rate of the Penalty Function Method, Z. Vycisl. Mat. i Mat. Fiz., Vol. 11, pp. 3-11.

Powell, M. J. D. (1969). A Method for Nonlinear Constraints in Minimization Problems, in Optimization, R. Fletcher, ed., Academic Press, New York, pp. 283-298.

Powell, M. J. D. (1977). A Fast Algorithm for Nonlinearly Constrained Optimization Calculation. Report CAMTP 77/HA 2, Cambridge University, England.

Rockafeller, R. T. (1973). A Dual Approach to Solving Nonlinear Programming Problems by Unconstrained Optimization, Math Programming, Vol. 5, pp. 354-373.

Tapia, R. A. (1971). The Differentiation and Integration of Nonlinear Operators, in Nonlinear Functional Analysis and Applications, L. B. Rall, ed., Academic Press, New York.

Tapia, R. A. (1977). Quasi-Newton Methods for Equality Constrained Optimization: Equivalence of Existing Methods and a New Implementation, in Nonlinear Programming 3, O. Mangasarian, R. Meyer and S. Robinson, (eds.), Academic Press, New York, pp. 125-164.

Tapia, R. A. (1979). Augmented Lagrangian Methods for Constrained Optimization: The Role of the Penalty Constant, in Ottimizzazione non Lineare e Applicezioni, Incerti, S and Treccani, G. (eds.), Pitagora Editrice, Bologna, Italy, pp. 161-186.

Tapia, R. A. (1980). On the Role of Slack Variables in Quasi-Newton Methods for Constrained Optimization, in Numerical Optimization of Dynamic Systems, L. C.W. Dixon and G. P. Szego (eds.), North Holland, Amsterdam, pp. 235-246.

Zangwill, W. I. (1967). Non-linear Programming via Penalty Functions, Management Science, Vol. 13, pp. 344-358.