Convergence Analysis for a Multiplier-Free Reduced Hessian Method

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CONVERGENCE ANALYSIS FOR A MULTIPLIER FREE REDUCED HESSIAN METHOD

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We propose a quasi-Newton algorithm for solving optimization problems with nonlinear equality constraints. It is designed for problems with few degrees of freedom and does not require the calculation of Lagrange multipliers. It can also be extended to large-scale systems through the use of sparse matrix factorizations. The algorithm has the same superlinear and global properties as the reduced Hessian method developed in our previous paper (Biegler, Nocedal and Schmid, 1995). This report directly reworks the theory presented in that paper to consider the multiplier free case.

1. Introduction.

We consider the nonlinear optimization problem

$$\underset{x\in\mathbf{R}^n}{\mathrm{mim}}/(x) \qquad (1.1)$$

$$\text{subject to } \; c(x) = 0, \qquad (1.2)$$

where / : R^n —• R and c : R^n —> R^m are smooth functions. We assume that the first derivatives of / and *c* are available, but our algorithm does not require second derivatives. The successive quadratic programming (SQP) method for solving (1.1)-(1.2) generates, at an iterate #*, a search direction d_k by solving

$$\min_{d\in\mathbf{R}^n} \; g(x_k)^T d + \backslash d^T W\{x_k)d \qquad (1.3)$$

$$\text{subject to } \; c(x_k) + A\{x_k)^T d = 0, \qquad (1.4)$$

where *g* denotes the gradient of /, *W* denotes the Hessian of the Lagrangian function L(x, A) = *f(x)* + A^Tc(x), and *A* denotes the n x m matrix of constraint gradients

$$A(x) = [\nabla c_1(x), ..., \nabla c_m(x)]. \qquad (1.5)$$

A new iterate is then computed as

$$x_k+\backslash = x_k + a_k d_k, \qquad (1.6)$$

where a_k is a steplength parameter chosen so as to reduce the value of the merit function. In this study we will use the $t\backslash$ merit function

$$\wedge(x) = /(x) + _M||c(x)||_1, \qquad (1.7)$$

where /i is a penalty parameter; see for example Conn (1973), Han (1977) or Fletcher (1987). This penalty parameter is normally based on Lagrange multiplier values or their estimates but here we consider a simpler measure that does not require Lagrange multiplier estimates, but still maintains descent properties for *(fi^x).*

The solution of the quadratic program (1.3)-(1.4) can be written in a simple form if we choose a suitable basis of R^n to represent the search direction d_k. For this purpose, we introduce a nonsingular matrix of dimension n, which we write as

$$[Y_k Z_k], \qquad (1.8)$$

where Y_k *e* $R^{n \times m}$ and Z_k € $R«^x(^n-^m)$, and assume that

$$AlZ_k = 0. \qquad (1.9)$$

(From now on we abbreviate $A(x_k)$ as A_k, $g(x_k)$ as g_k, etc.) Thus Z_k is a basis for the tangent space of the constraints. We can now express d_k, the solution to (1.3)-(1.4), as

$$d_k = Y_k p_Y + Z_{kPz}, \qquad (1.10)$$

for some vectors p_Y € R^m and p_z € $R^n{\sim}^m$. Due to (1.9) the linear constraints (1.4) become

$$c_k + AlY_k p_Y = 0. \qquad (1.11)$$

If we assume that *Ak* has full column rank then the nonsingularity of *[Yk Zk]* and equation (1.9) imply that the matrix $A^\wedge Y_k$ is nonsingular, so that p_Y is determined by (1.11):

$$p_Y = -[A_k^T Y_k]^{-1} c_k. \qquad (1.12)$$

Substituting this in (1.10) we have

$$d_k = -Y_k[AlY_h]^{-1}Ck + Z_{kPz}. \qquad (1.13)$$

The SQP sub-problem can now be expressed exclusively in terms of the variables p_z. Substituting (1.10) into (1.3), considering $Y_k p_Y$ as constant, and ignoring constant terms, we obtain the unconstrained quadratic problem

$$\min_{p_Z \in \mathbf{R}^{n-m}} (Z_k^T g_k + Z_k^T W_k Y_k p_Y)^T p_Z + \backslash\, p_Z{}^T (Z_k^T W_k Z_k) p_Z. \quad 1 \quad 4 \quad)$$

Assuming that $Z\%W_kZ_k$ is positive definite, the solution of (1.14) is

$$p_z = -(Zl\ W_k[Z_kZ)^{-l}\ g\ _k\ +\ ZlW_kY_kp_Y). \qquad (1.15)$$

This determines the search direction of the SQP method.

In our previous paper (Biegler, Nocedal and Schmid, 1995) the cross term $[Z^T{}_kW_kY_k\backslash p_Y$ is approximated by a vector it;*,

$$[ZlW_kY_k]p_Y{*}w_k, \qquad (1.16)$$

without computing the matrix $Z\%W_kY_k$. This allows the rate of convergence of the algorithm to be 1-step Q-superlinear, as opposed to the 2-step superlinear rate for methods that ignore the cross term (Byrd (1985) and Yuan (1985)). The null space step (1.15) of our algorithm will be given by

$$p_z\ =\ -\{ZlW_kZ_k)^{-l}[Zlg_k\ +\ (_kw_k), \qquad (1.17)$$

where $0 < (_k \leq 1$ is a damping factor described in our previous paper.

Here the cross term is approximated either by a finite difference estimate along Y_kp_Y or by a quasi-Newton method in which the rectangular matrix $Z\wedge W_k$ is approximated by a matrix S_k, using Broyden's method. We then obtain w_k by multiplying this matrix by Y_kp_Y, i.e.,

$$w_k\ =\ S_kY_kp_Y.$$

In this study, we update $S_k+\backslash$ so that it satisfies the following secant relation:

$$S_k+i(x_M\ -\ x_k)\ =\ Zl+_{l9}(x_k+i)\ -\ Zlg\{x_k). \qquad (1.18)$$

Let us now consider how to approximate the reduced Hessian matrix $Z\wedge W_kZ_k$. Prom (1.6), (1.10) and (1,18) we obtain

$$[S_k+iZ_k]a_kp_z\ =\ -a_kS_k+i(Y_kp_Y)\ +\ Z\wedge gixk+i)\ -\ Zlg(x_k).$$

Since $S_k+\backslash$ approximates Z^TW, this suggests the following secant equation for 27&+1, the quasi-Newton approximation to the reduced Hessian Z^TWZ:

$$B_{k+1}s_k = y_k, \qquad (1.19)$$

where s_k and y_k are defined by $s_k \doteq a_kp_z$, and

$$Vk\ =\ ZZ+_{l9}(x_k+0\ -\ Zlg\{x_k)\ -\ \overline{w}_k, \qquad (1.20)$$

with

$$W_k\ =\ a_kS_M(Y_kp_Y). \qquad (1.21)$$

We will update B_k by the BFGS formula (cf. Fletcher (1987))

$$B_{k+1} = B_k - \frac{B_ks_ks_k^TB_k}{s_k^TB_ks_k} + \frac{y_ky_k^T}{y_k^Ts_k}, \qquad (L22)$$

provided s^y* is sufficiently positive. As a result, the null space step is computed from:

$$B_k P z = -\{Z k^T 9 k + OfcUfc) \qquad (1.23)$$

Note as in our previous paper, that two correction terms, *Wk* and *Wk* are applied. The first term, *Wk,* is used in the null space step (1.23) and makes Use of the matrix 5*. The second term, *Wk* is used in (1.20) for the BFGS update of *Bk* and is computed using the new Broyden matrix 5fc+i, and takes into account the steplength a*. We will see below that it is useful to incorporate the most recent information in *Wk-*

Finally, as noted by Orozco (1993), an interesting relationship in the definition of basis representations and Lagrange multipliers occurs for a particular choice of *Z* and *Y,* If we define the Lagrange multiplier estimates by:

$$A(x) = -[YixfAixT'Yixfgix). \qquad \bullet\ (1.24)$$

and partition *x* into m basic or dependent variables (which without loss of generality are assumed to be the first m variables) and *n — m* nonbasic or control variables, we induce the partition

$$A(x)^T = [C(x)N(x)\}, \qquad (1.25)$$

where the *m* x *m* basis matrix *C(x)* is assumed to be nonsingular. We now define *Z(x)* and *Y{x)* to be

$$ZW\bullet \ [-*«;'*« \ ]\ y(,,\bullet[j]. \qquad (1.26)$$

This choice is particularly advantageous when *A(x)* is large and sparse, because a sparse LU decomposition of *C{x)* can often be computed efficiently, and this approach will be considerably less expensive than a QR factorization of *A(x).* It is also straightforward to show that for any points $\overline{x}$, $\hat{x}$ for which $C(\overline{x})$, $C(\hat{x})$ are nonsingular, we have

$$Z(\hat{x})^T VL(x,\overline{\ }(x)) = Z(\overline{x})^T g(\overline{x}) \qquad (1.27)$$

This allows us to make the following equivalence in the calculation of %.

$$\begin{aligned} Vk &= Zl+_x g\{xk+\backslash)-Zlg\{x_k)-v\overline{5}_k \\ &= ZjVL(z^*+i,\ A_{fc+}i) - Zj[g\{x_k) - W_k \end{aligned} \qquad (1.28)$$

when (1.26) is chosen for *Y* and Z.

In the next section we discuss the revised reduced Hessian algorithm in detail. In particular, we briefly describe the calculation of the correction terms w_k and *Wf^* the conditions under which BFGS updating takes place, the choice of the damping parameter Ok, and the procedure for updating the weight fi_k in the merit function. Most of these steps are identical to the ones in our previous paper. Section 3 presents an analysis of the local behavior of the algorithm, shows that the rate of convergence is at least R-linear and summarizes the properties related to superlinear convergence. Numerical results and extensions to consider variable bounds are described in a companion paper (Biegler, Schmid and Ternet, 1995).

Regarding our notation, throughout the paper the vectors p_Y and p_z are computed at Zfc, and could be denoted by p_Y^ and p_z^^{k}\ but we will normally omit the superscript for simplicity. The symbol || • || denotes the *I2* vector norm or the corresponding induced matrix norm. When using the *l*\ or /<» norms we will indicate it explicitly by writing II • 111 **or** || • Hoc. A solution of problem (1.1) is denoted by x*, and we define

$$e_k = x_k - x+ \quad \text{and} \quad a_k = \mathbf{max\{||e*||,} \; ||e*+i||\}. \tag{1.29}$$

2. Details of the Multiplier-Free Algorithm

In this section we consider[1] how to calculate approximations w_k and $\overline{w}_k$ to *(Z%W$_k$Y$_k$)p$_Y$* to be used in the determination of the search direction p_z and in updating 2?*, respectively. We also discuss when to skip the BFGS update of the reduced Hessian approximation, as well as the selection of the damping factor *Ck* and the penalty parameter /i&.

To approximate to *(Z^{T}WY)p$_Y$* we propose two approaches that have slight modifications to those proposed in our earlier paper. First, we consider a finite difference approximation to *Z][W$_k$* along the direction *Y$_k$p$_Y$*. The second approach defines w_k and $\overline{w}_k$ in terms of a Broyden approximation to *Z%W$_k$*, as discussed in §1, and requires no additional function or gradient evaluations. Our algorithm will normally use this second approach, although it is sometimes necessary to use finite differences.

2.1. Calculating w_k and $\overline{w}_k$ Through Finite Differences.

We first calculate the range space step p_Y at x_k through equation (1.12). Next we compute the reduced gradient of the Lagrangian at $x_k + Y_k p_Y$ and define

$$w_k = Z(x_k + Y_k p_Y fg(x_k + Y_k p_Y) - Zlg_k. \tag{2.1}$$

After the step to the new iterate x_k+\ has been taken, we define

$$\overline{w}_k = a_k w_k \tag{2.2}$$

which requires a new evaluation of gradients if a_k ^ 1. These correction terms are substituted for the ones used in our previous paper:

$$w_k = Zl[VL\{x_k + \mathbf{Y_{kPYy}} X_k) - VL(x_k,\backslash_k)]. \tag{2.3}$$

$$\overline{w}_k = Zl\backslash VL\{x_k + a_k Y_k p_Y, X_M) - VL\{x_k, A*_{+1})] \tag{2.4}$$

2.2. Using Broyden's Method to Compute w_k and $\overline{w}_k$.

We can approximate the rectangular matrix *Z^W$_k$* by a matrix 5* updated by Broyden's method, and then compute w_k and $\overline{w}_k$ by post-multiplying this matrix by $Y_k p_Y$

or by a multiple of this vector. As discussed in §1 it is reasonable to impose the secant equation (1.18) on this Broyden approximation, which can therefore be updated by the formula (cf. Fletcher (1987))

$$S_W \wedge g_{fc} + \frac{(fe" ; |ft)}{{}^s k^s k} \wedge \tag{2.5}$$

where

$$\bar{V}k = Zjf_+i0(s^*+i) - Zlg(x_k) \tag{2.6}$$

$$Sk = Zifc+i - x_k. \tag{2.7}$$

thus, defining

$$w_k = S_k Y_k p_Y \quad \text{and} \quad \overline{w}_k = a_k S_k + iY_k p_Y. \tag{2.8}$$

As in our previous paper, we apply a safeguard on these updates to make sure that w_k and $\overline{w}_k$ remain bounded. At the beginning of the algorithm we choose a positive constant T and define

$$w_k := \begin{cases} w_k & \text{if } \|w_k\| \leq \frac{\Gamma}{\|p_Y\|^{1/2}}\|p_Y\| \\ w_k \frac{\Gamma\|p_Y\|^{1/2}}{\|w_k\|} & \text{otherwise.} \end{cases} \tag{2.9}$$

On the other hand, the correction $\overline{w}_k$ will be safeguarded by choosing a sequence of positive numbers $\{7^*\}$ such that E-g1^ < 00, and set

$$\overline{w}_k \quad \begin{cases} \overline{w}_k & \text{if } \|\overline{w}_k\| \leq \alpha_k\|p_Y\|/\gamma_k \\ \overline{w}_k \frac{\alpha_k\|p_Y\|}{\gamma_k\|\overline{w}_k\|} & \text{otherwise.} \end{cases} \tag{2.10}$$

As the iterates converge to the solution, $p_Y \to 0$, we see from (2.8) and from the boundedness of Y_k that these safeguards allow the Broyden updates S_k to become unbounded, but in a controlled manner. In our previous paper, it was shown that these Broyden updates S_k do, in fact, remain bounded, so that the safeguards become inactive asymptotically.

2.3. Update Criterion.

It is well known that the BFGS update (1.22) is well defined only if the curvature condition $s^\wedge y_k > 0$ is satisfied. This condition can always be enforced in the unconstrained case by performing an appropriate line search; see for example Fletcher (1987). However when constraints are present the curvature condition $s\% y_k > 0$ can be difficult to obtain, even near the solution.

To show this we first note from (1.20), (1.10) and from the Mean Value Theorem that

$$\begin{aligned} y_k &= Z\% + xgfc{+}i \sim Z_k^T g_k - \overline{w}_k \\ &= Z_{k+1}^T \nabla L(x_{k+1}, \lambda_*) - Z_k^T \nabla L(x_k, \lambda_*) - \overline{w}_k \\ &= Zl \left[\int^1 V^2_{xx} L\{x_k + r a_k d_k, \backslash^*) dr \right] a_k d_k + (Z_{fc+}i - Z_k)^T VL(x_k +_u K) - \overline{w}_k \\ &\equiv Zl\tilde{W}_k a_k d_k + (Z^*{}_+i - Zib)^r VL(xfc_+i, A^*) - \overline{w}_k \\ &= Z_j^{\prime} F\tilde{W}_k Z_k s_k + O(a^\wedge\|s_k\| + \alpha_k\|p_Y\|) + \alpha_k Z_k^T \tilde{W}_k Y_k p_Y - \overline{w}_k, \end{aligned} \tag{2.11}$$

where we have defined

$$Z_k^T \tilde{W}_k = Zl \int_{Jo}^{1} V^2_{xx} L\{x_k + Ta_k d_k, X.)dr. \tag{2.12}$$

Thus

$$sly_k = s^T{}_k\{Zl\bar{W}_k Z_k)s_k + O(a_k)\|_{Sk}f + [a_k sj\,(ZjW_k\tilde{Y}_k)p_Y - \#57^*] + O(o_k)\|a_k\|\ \|py\,\|. \tag{2-13}$$

Near the solution, the two O(a&) terms will vanish, while the first term on the right hand side will be positive since *Z^W^Zk* can be assumed positive definite. Nevertheless the bracketed terms in (2.13) are of uncertain sign and can make *s^yk* negative. To avoid this problem and also ensure that the quasi-Newton approximation remains boimded, we apply the same updating criterion developed in our previous paper.

Update Criterion I.

Choose a constant $y_{\{d}$ > 0 *and a sequence of positive numbers {jk} such that* Ej^^fc < oo *(this is the same sequence* {7*} *that was used in (2.10)).*

- *IfWk is computed by Broyden's method, and if both s^yk* > 0 *and*

$$\mathbf{Ibvll \le 7^{*2}IM} \tag{2.14}$$

hold at iteration k, then update the matrix Bk by means of the BFGS formula (1.22) with Sk and y* *given by (1.20). Otherwise, set* $B_{k+1} = B_k$.

- *// Wk is computed by finite differences, and if both s£yk* > 0 *and*

$$\|p_Y\| \le \gamma_{fd}\|p_Z\|/\sigma i^{/2} \tag{2.15}$$

hold at iteration k, then update the matrix Bk by means of the BFGS formula (1.22) with Sk and yk given by (1.20). Otherwise, set Bk+i = Bk.

Here *Ok* is replaced by any quantity which is of the same order as the error e*, and, as in our previous paper, we use the optimality condition (IIZjjTitell + ||cfc||). Moreover, define

$$\cos\theta_k = \frac{s_k^T B_k s_k}{\|s_k\|\,\|B_k s_k\|}. \tag{2.16}$$

Prom Byrd and Nocedal (1989), the behavior of cos0* for BFGS updates can be described by the following theorem.

Theorem 2.1 *Let {B_k} be generated by the BFGS formula (1.22) where, for all k>\, Sk ^0 and*

$$\frac{\%^T\!\wedge}{s_k^T s_k} \ge m > 0 \tag{2.17}$$

$$\frac{\|y_k\|^2}{y_k^T s_k} \le M. \tag{2.18}$$

Then, there exist constants /3\, 02,03 > **0** *such that, for any* $k \geq 1$, *the relations*

$$\cos Oj \ \geq \ fa \tag{2.19}$$

$$\beta_2 \leq \frac{\|B_j s_j\|}{\|s_j\|} \leq \beta_3 \tag{2.20}$$

hold for at least **f^fc]** *values of j* **€ [l,fc].**

This theorem refers to the iterates for which BFGS updating takes place, but since for the other iterates *Bk*+\ = £*, the theorem characterizes the whole sequence of matrices {£fc}. Theorem 2.1 states that, if s^y* is always sufficiently positive, in the sense that conditions (2.17) and (2.18) are satisfied, then at least half of the iterates at which updating takes place are such that *cosOj* is bounded away from zero and *BjSj* = O(||SJ||). Since it will be useful to refer easily to these iterates, we make the following definition.

Definition 2,1 *We define J to be the set of iterates for which BFGS updating takes place and for which (2.19) and (2.20) hold. We call J the set of "good iterates'*[7]*, and define* J_k = **Jfl {1,2,...,A;}.**

Note that if the matrices *Bk* are updated only a finite number of times, their condition number is bounded, and (2.19)-(2.20) are satisfied for all fc. Thus in this case all iterates are good iterates.

For the case when BFGS updating takes place an infinite number of times, we assume that all functions under consideration are smooth and bounded. If at a solution point x* the reduced Hessian $ZjW{+}Z_m$ is positive definite, then for all x_k in a neighborhood of *x the smallest eigenvalue of *Z^W^Zk* is bounded away from zero *(W^* is defined in (2.12)). We now show that in such a neighborhood with a* sufficiently small that Update Criterion I implies (2.17)-(2.18). For the case when $\overline{w}$^ is computed by Broyden's method. Using (2.13), (2.14) and (2.10), and since 7* converges to zero, we have**

$$\begin{aligned} s_k^T y_k &\geq C\|s_k\|^2 - O(\gamma_k^2\|s_k\|^2) - O(\gamma_k\|s_k\|^2) \\ &\geq m\|s_k\|^2, \end{aligned} \tag{2.21}$$

for some positive constants *C,m.* Also, from (2.11), (2.14) and (2.10) we have that

$$\begin{aligned} \|y_k\| &\leq O(\|s_k\|) + O(\gamma_k^2\|s_k\|) + O(\gamma_k\|s_k\|) \\ &\leq O(\|s_k\|). \end{aligned} \tag{2.22}$$

We thus see from (2.21)-(2.22) that there is a constant *M* such that for all *k* for which updating takes place

$$\frac{\|y_k\|^2}{y_k^T s_k} \leq M,$$

which together- with (2.21) shows that (2.17)-(2.18) hold when Broyden's method is used.

For $\overline{w}_k$ computed by the finite difference formula (2.2), from (1.20) and the Mean Value theorem there is a matrix $\hat{W}_k$ such that

$$
\begin{aligned}
y_k &= Z_{k+1}^T g_{k+1} - Z_k^T g_k - \overline{w}_k \\
&= Z_{k+1}^T \nabla L(x_{k+1}, \lambda_*) - Z_k^T \nabla \\
&\quad L(x_k, A_t) - a_k[Z_{(}x_k + Y_{kPY})^T VL\{x_k + Y_k p_Y, A.) - 2\% VL(x_k, A.)] \\
&= (Z_{fc+}i - Z_k)^T VL(x_{k+1}, A.) + Zl(VL(x_{fc+}i, A,) - VL(s^*, A,)) \\
&\quad -\alpha_k[(Z_{(}x_k + Y_k p_Y) - Z_k)^T VL(x_k + Y_k p_Y, A.) \\
&\quad + Z_k^T(\nabla L(x_k + Y_k p_Y) A.) - VX(x_{fc}, A.))] \\
&= Zl\tilde{W}_k Z_k s_k + a_k Zl(\tilde{W}_k - \hat{W}_k) Y_{kPy} + O(a_k) \|s_k\| \\
&= Z_k^T \tilde{W}_k Z_k s_k + O\{a_k)\|s_k\|.
\end{aligned}
$$

assuming $Y_k py = 0\{a_k)$. Reasoning as before we see that (2.21) and (2.22) also hold in this case, and that (2.17)-(2.18) are satisfied in the case when finite differences are used. These arguments show that, in a neighborhood of the solution and whenever BFGS updating of B_k takes place, $s\backslash y_k$ is sufficiently positive, as stipulated by (2.17)-(2.18).

2.4. A Multiplier-free Approach for Choosing n_k.

We will choose $\backslash i$ so that for some $p > 0$,

$$MH^*)\|\geq|A(^*)M^*)|+p\|c(^*)\| \tag{2.23}$$

and show that this approach ensures a descent direction for the merit function. Moreover, for the good iterates J, it is a direction of strong descent.

Since d^ satisfies the linearized constraint (1.11) it is easy to show (see eq. (2.24) of Byrd and Nocedal (1991)) that the directional derivative of the $l\backslash$ merit function in the direction d* is given by

$$D\wedge_k(x_k;d_k) = gld_k - \text{WfclMlx}. \tag{2.24}$$

Also, the fact that the same right inverse of $A(x)^T$ is used in (1.12) and (1.24) implies that

$$g(x)^T Y(x) p_Y = \backslash(x)^T c(x). \tag{2.25}$$

We now show the following relation between Kuhn-Tucker points and merit functions with /i chosen by (2.23).

Theorem 2,1 *Assume that A(x) is of full column rank for all x € D and that Z(x) is norm bounded. If (p^x) is defined by (1.7) and fx satisfies (2.23) for all x* G *D, then D<t>7\{x\d) > 0 for all d satisfying $\bar{c}(x) + \bar{A}(x)^T d = 0$ if and only if $\bar{x}$ is a Kuhn-Tucker point.*

Proof. The proof is similar to the one in Fletcher (1987) for <£M(x) with /i > $\|\lambda(\bar{x})\|_\infty$. The *if part* follows from:

$$
\begin{aligned}
0 \le D\phi_\mu(\bar{x};d) &= \bar{g}(xfd\text{-}n\backslash\backslash c(\bar{x})\backslash\backslash i \\
&= g\{x)^T Z(\bar{x})p_z\text{-}_f x\backslash\backslash c(x)\backslash\backslash_1 + X\{\bar{x})^T c(\bar{x}) \\
&\le \bar{g}(x)^T \bar{Z}(x)p_z\text{-}p\backslash\backslash c(\bar{x})\backslash\backslash i \\
&\le g(\bar{x})^T Z(\bar{x})p_z \qquad (2.26)
\end{aligned}
$$

for all p_z € $H^n\sim^m$. This implies $Z(\bar{x})^T g\{x)^- = 0$. Now if, in addition, $c(\bar{x}) = 0$ then $\bar{x}$ is a Kuhn-Tucker point. If we assume $c(\bar{x})$ ^ 0 then we can show the contradiction:

$$
\begin{aligned}
0 \le Z\%(\bar{x};d) &= \backslash\{x)^T c(\bar{x}) - /i||c(2)||i \\
&\le -p||c(S)||i- \\
&< 0. \qquad (2.27)
\end{aligned}
$$

The *only if* part follows from substitution of the Kuhn-Tucker conditions:

$$
\begin{aligned}
Z(\bar{x})^T g(\bar{x}) &= 0 \\
c(\bar{x}) &= 0 \qquad (2.28)
\end{aligned}
$$

into the directional derivative:

$$
\begin{aligned}
D\text{^}(x;\bar{<}f) &= \bar{g}(x)^T Z(x)_{Pz}\text{-}fjL\backslash\backslash\bar{c}(x)\backslash\backslash iHx)^T c(\bar{x}) \\
&= 0. \qquad (2.29)
\end{aligned}
$$

D

To show strong descent directions for good iterates, we recall the decomposition (1.23) and use (2.25) to obtain

$$
\begin{aligned}
D\phi_{\mu_k}(x_k;d_k) &= g_k^T Z_k p_z - \mu_k\|c_k\|_1 + \lambda_k^T c_k \\
&= (Z_k^T g_k + \zeta_k w_k)^T p_z - \zeta_k w_k^T p_z - \mu_k\|c_k\|_1 + \lambda_k^T c_k. \qquad (2.30)
\end{aligned}
$$

Now from (1.23) we have that

$$BkSk = —OL_k(Z_k^T g_k + \text{Cifc^A:)-} \qquad (2.31)$$

As shown in our previous paper,

$$\cos\theta_k = \frac{-(ZZgk + \{kWk)^T Pz}{\backslash\backslash 2\%gk + tkWk\backslash\backslash\backslash\backslash Pz\backslash\backslash'} \qquad (2.32)$$

If we satisfy the following property for fi_k:

$$H_k\backslash\backslash c_k\backslash\backslash \ge \backslash Xlc_k\backslash + 2p\backslash\backslash c_k\backslash\backslash \qquad (2.33)$$

or, equivalently, from (2.25):

Wfellc*ll $\geq$ *igjYkPvl + 2p\\ck* **(2.34)**

then substituting in (2.30), leads to:

$$D\phi_{\mu_k}(x_k; d_k) \leq -\|Z_k^T g_k + \zeta_k w_k\| \, \|p_z\| \cos\theta_k - \zeta_k w_k^T p_z - 2\rho\|c_k\|_1. \tag{2.35}$$

Note also from (2.31) that

$$\frac{\text{11**11}}{\|B_k s_k\|} = \frac{\text{lift 11}}{\|Z_k^T g_k + \zeta_k w_k\|}. \qquad \text{(2.3gX)}$$

We now concentrate on the good iterates J, as given in Definition 2.1. If *j* G J, we have from (2.36) and (2.20) that

$$\frac{1}{\beta_3}\|Z_j^T g_j + \zeta_j w_j\| \leq \|p_z^{(j)}\|, \text{ - } \frac{1}{\mu_2} \text{ir}\backslash\backslash^{Z} i\ 9j\ +\ CjWjll \tag{2.37}$$

Using this and (2.19) in (2.35) we obtain, for *j* 6 *J*,

$$D\phi_{\mu_j} ix_j d\ _j) \leq -\frac{1}{\beta_3}\ \backslash\backslash Zg_j\ + \zeta_j w_j\|^2 \cos\theta_j - \zeta_k w_j^T p_z^{(j)} - 2\rho\|c_j\|_1$$

$$\leq\ \text{-}\wedge\backslash\backslash zj_{9j}f\ \text{-}\ \ ^2 Si\wedge i_{\{g} T_{ZjWj)}\ \ - CjWj_{P}\mu)\ - mej\ \|_1,$$

where we have dropped the non-positive term — *tf cosQJ\\WJ*^{2}*/fa.* Since we can assume that /% > 1 (it is defined as an upper bound in (2.20)), we have

$$D\phi_{\mu_j}(x_j; d_j) \leq -f y\ \|Z_j^T g_j\|^2 + \ \zeta_j \cos\theta_j |g_j^T Z_j w_j| - 2\rho\|c_j\|_1 - \zeta_j w_j^T p_z^{(j)}$$

It is now clear that if

2Cj cos *6j\gjZjWj*| - *CjwjpV** $\leq$ *p\\cj* ||i, **(2.38)**

then for all *j* G J,

DϕH(xy,dj) $\leq$ - ^ l l ^ l l ^{2} - ***pWcjh.*** **(2.39)**

This means that if (2.38) holds, then for the good iterates, *j* € J, the search direction *dj* is a strong direction of descent for the *t* merit function in the sense that the first order reduction is proportional to the KKT error.

We will choose £* so that (2.38) holds for *all* iterations. To see how to do this we note from (1.23) that

$$p_z = -B_k^{-1} Z_k^T g_k - \zeta_k B_k^{-1} w_k,$$

so that for $j = k$ (2.38) can be written as

$$Ck[2cos6_k\backslash glZ_kw_k\backslash + w^T{}_kBl^xZlg_k + CkwlB\wedge^lw_k] \leq p||c_{fc}||i. \qquad (2.40)$$

It is clear that this condition is satisfied for a sufficiently small and positive value of £*. Specifically, at the beginning of the algorithm we choose a constant $p > 0$ and, at every iteration fc, define

$$Œ = \min\{l, C\hat{f}c\} \qquad (2.41)$$

where $\hat{0}t$ is the largest value that satisfies (2.40) as an equality.

The penalty parameter /z* must satisfy (2.23), so we define it at every iteration of the algorithm by

$$\mu_k = \begin{cases} \mu_{k-1} & \text{if } \mu_{k-1}\|c_k\|_1 \geq |g_k^T Y_k p_Y| + 2\rho\|c_k\|_1 \\ |g_k^T Y_k p_Y|/\|c_k\|_1 + 3\rho & \text{otherwise.} \end{cases} \qquad (2.42)$$

Note that for $c_k = 0$ μ_k = /Zfc_i and thus fx_k is only updated when $c_k \wedge 0$.

The damping factor £* and the updating formula for the penalty parameter fi_k have been defined so as to give strong descent for the good iterates J. We now show that they ensure that the search direction is also a direction of descent (but not necessarily of strong descent) for the other iterates, k & J. Since (2.38) holds for all iterations by our choice of Œ> we have in particular

$$-\zeta_k w_k^T p_Z \leq \rho\|c_k\|_1.$$

Using this and (2.42) in (2.35), we have

$$D\phi_{\mu_k}(x_k; d_k) \leq -\|Z_k^T g_k + \zeta_k w_k\| \, \|p_Z\| \cos\theta_k - \rho_k\|c_k\|_1. \qquad (2.43)$$

The directional derivative is thus non-positive. Furthermore, since $w_k = 0$ whenever $c_k = 0$ (regardless of whether w_k is obtained by finite differences or through Broyden's method), it is easy to show that this directional derivative can only be zero at a stationary point of problem (1.1)-(1.2).

2.5. The Algorithm

- Using the modifications of the reduced Hessian algorithm for the multiplier-free method, we now give a complete description of the algorithm. As with the previous paper, the algorithm includes an approximation for the cross term using Broyden's method and finite differences, and based on the relative sizes of p_Y and p_Z. Calculation of the cross term and updating of the reduced Hessian proceed in the same manner as in our previous paper.

Algorithm I

1. Choose constants 77 E (0,1/2), $p > 0$ and r,r^f with $0 < r < r' < 1$, and positive constants F and j_{id} for conditions (2.9) and (2.15), respectively. For conditions (2.10) and (2.14), select a summable sequence of positive numbers {7*}. Set $k := 1$ and choose a starting point xi, an initial value .(JL\ > 0 for the penalty parameter, an (n — *m)* x (n — *m)* symmetric and positive definite starting matrix *B* and an *(n — m) x n* starting matrix *S*.

2. Evaluate /*,</*, c* and *Ak,* and compute % and Z*.

3. Set *findiff* = *false* and compute p_Y by solving the system

$$(AlY_k)p_Y = -c*. \qquad \text{(range space step)} \qquad (2.44)$$

4. Calculate tu* using Broyden's method, from equations (2.8) and (2.9).

5. Choose the damping parameter *C,k* from equations (2.40) and (2.41) and compute p_z from

$$B_k p_z = -\backslash^z k9^T k + CkWk]- \qquad \text{(null space step)} \qquad (2.45)$$

6. If (2.15) is satisfied and (2.14) is *not* satisfied, set *findiff* = *true* and recompute *Wk* from equation (2.1).

7. If *findiff* = *true* use this new value of *w^* to choose the damping parameter £* from equations (2.40) and (2.41) and recompute p_z from equation (2.45).

8. Define the search direction by

$$d_k = Y_k p_Y + \text{Zfcp}_z, \qquad (2.46)$$

and set a& = 1.

9. Test the line search condition

$$<t>n_k(xk + <*kdk) \leq <l>n_k\{xk) + vakDcfr\wedge ixkidk). \qquad (2.47)$$

10. If (2.47) is not satisfied, choose a new a* E *[rak,r'ak]* and go to 9; otherwise set

$$\text{Xfc+i}\wedge\text{fc} + \text{afcd*}. \qquad (2.48)$$

11. Evaluate /*+i,0*4.1,c*+i, $A*_{+}$i, and compute Yjk4i and Z*+i.

12. Update /x* so as to satisfy (2.42).

13. Update £*+! using equations (2.5) to (2.7). If *findiff* = *false* calculate tJ* by Broyden's method through equations (2.8) and (2.10); otherwise calculate *Wk* by (2.2).

14. If $s\%y_k \leq 0$ or if (2.15) is not satisfied, set -B^+i = B_k. Else, compute

$$s^* = <**Pz, \tag{2.49}$$

$$Vk = Zl+_{ig}\{x_k+i) - Zlg\{x_k) - \overline{w}_k, \tag{2.50}$$

and compute $B_k +_X$ by the BFGS formula (1.22).

15. Set A; := k + 1, and go to 3.

3. Convergence Results

In this section we summarize several convergence results for Algorithm I. Many of the results of the our previous paper carry over directly and are thus stated without proof. Nevertheless, there are some important departures which are noted as well.

3.1. Semi-Local Behavior of the Algorithm.

We first show that the merit function <*f*>^ decreases significantly at the good iterates J, and that this gives the algorithm a weak convergence property. To establish the results of this section we restate the following assumptions from our previous paper.

Assumptions 3.1 The sequence $\{x_k\}$ generated by Algorithm I is contained in a convex set D with the following properties.

(I) The functions / : R^n -> R and c : R^n -* R^m and their first and second derivatives are uniformly bounded in norm over D.

(II) The matrix $A(x)$ has full column rank for all x € D, and there exist constants 70 and *fa* such that

$$WYixnAixfYix)\}-^1\wedge\wedge, \qquad ||Z(s)||<\underline{i}flb, \tag{3.1}$$

for all x € D.

(III) For all $k \geq 1$ for which B_k is updated, (2.17) and (2.18) hold.

(IV) The correction term to* is chosen so that there is a constant K > 0 such that for all

$$\|w_k\| \leq KllcfeU^1/^2. \tag{3.2}$$

The following result from our previous paper concerns the good iterates J, as given in Definition 2.1.

Lemma 3.1 *If Assumptions 3.1 hold and if fij = fj, is constant for all sufficiently large j, then there is a positive constant* 7^ *such that for all large j* G J,

$$\phi_\mu(x_j) - \phi_\mu(x_{j+1}) \geq 7M\,[11\hat{}j11^2 + IMh] \bullet \tag{3.3}$$

It is now easy to show that the penalty parameter settles down, and that the set of iterates is not bounded away from stationary points of the problem.

Theorem 3.2 *If Assumptions 3.1 hold, then the weights* {/x/k} *are constant for all sufficiently large k and]imM$_k$->oo(\\ZTk 9k* + l|c*ll) = 0.

Proof. First note that by Assumptions 3.1 (I)-(II) and (2.25) that {Ilffjf1*p$_Y$|/||c*||i} = {|^jf^{c}fcl/ll^c*lli} ^ {11^*11} is bounded. Therefore, since the procedure (2.42) increases /U* by at least *p* whenever it changes the penalty parameter, it follows that there is an index fco and a value /i such that for all *k* > fco, Wb = A$^{4 suc}$h *kat Ml|c/k||i ≥ |A£cfc| + 2p||c*|ji. If BFGS updating is performed an infinite number of times, by Assumptions 3.1-(III) and Theorem 2.1 there is an infinite set *J* of good iterates, and by Lemma 3.1 and the fact that *<f>n(xk)* decreases at each iterate, we have that for *k* > &o,

$$\begin{aligned}
\phi_\mu(x_{k_0}) - \phi_\mu(x_{k+1}) &= \sum_{j=k_0}^{k} (\phi_\mu(x_j) - \phi_\mu(x_{j+1})) \\
&\geq \sum_{j \in J \cap [k_0,k]} (\phi_\mu(x_j) - \phi_\mu(x_{j+1})) \\
&\geq \gamma_\mu \sum_{j \in J \cap [k_0,k]} [\|Z_j^T g_j\|^2 + \|c_j\|_1].
\end{aligned}$$

By Assumption 3.1-(I) ^$_M$(x) is bounded below for all **x E D,** so the last sum is finite, and thus the term inside the square brackets converges to zero. Therefore

$$\lim_{j \in J} (P| j \wedge +1\wedge 110 = 0. \tag{3.4}$$

If BFGS updating is performed a finite number of times then, as discussed after Definition 2.1, all iterates are good iterates, and in this case we obtain the stronger result

.lim (H^ffjtH + Hcfclli) = 0.

□

3.2. Local Convergence

In this section we show that if *x+* is a local minimizer that satisfies the second order optimality conditions, and if the penalty parameter /x* is chosen large enough, then x* is a point of attraction for the sequence of iterates *{xk}* generated by Algorithm I. To prove this result we will make the following assumptions. In what follows *G* denotes the reduced Hessian of the Lagrangian function, i.e.

$$G_k = Z_k^T \nabla_{xx}^2 L(x_k, \lambda_k) Z_k. \tag{3.5}$$

Assumptions 3.2 The point z* is a local minimizer for problem (1.1)-(1.2) at which the following conditions hold.

(1) The functions / : R^n -> R and *c* : R^n -» R^m axe twice continuously differentiable in a neighborhood of x*, and their Hessians are Lipschitz continuous in a neighborhood **of x_*.**

(2) The matrix *A(x+)* has full column rank. This implies that there exists a vector A* G R^m such that

VL(z*, A,) = *g*(x_m) + *A{x*)** = 0.

(3) For all *q e* R^{n}~^{m}, *q* ^ 0, we have $q^T G_* q > 0$.

(4) There exist constants 70, /?o and 7_C such that, for all *x* in a neighborhood of x*,

WYixHAixfYix^WK-to, ***\\Z(x)\\≤f3o,*** **(3.6)**

and

\\[Y(x)Z(x)]-^{1}\\≤y_c. (3.7)

(5) *Z(x)* and *X(x)* are Lipschitz continuous in a neighborhood of x«, i.e. there exist constants j_z and 7^ such that

$$\|\lambda(x) - \lambda(z)\| \le \gamma_\lambda \|x - * II, \tag{3.8}$$

\\Z(x) - Z(z) ≤ $_7$z||x-z||, (3.9)

for all *x, z* near x».

Note that (1), (3) and (5) imply that for all *(x, X)* sufficiently near (x,,A»), and for all *q* € R$^{n"m}$,

m\\q\\$^2$≤q^{T}G(x,\)q<M\\q\\$^2$, (3.10)

for some positive constants m, M. We also note that Assumptions 3.2 ensure that the conditions (2.17)-(2.18) required by Theorem 2.1 hold whenever BFGS updating takes place in a neighborhood of x*. Therefore Theorem 2.1 can be applied in the convergence analysis.

The following lemma is proved by Xie (1991) for very general choices of *Y* and Z. Their result generalizes Lemma 4.1 of Byrd and Nocedal (1991); see also Powell (1978).

Lemma 3.3 *// Assumptions 3.2 hold, then for all x sufficiently near x**

$$\text{Till* - x.}|| \leq ||c(x)|| + \backslash\backslash Z\{x)^T g\{x)\backslash\backslash \lesssim {}_{l2}\backslash\backslash x - x.||, \quad (3.11)$$

for some positive constants 71,72 •

This result states that, near z*, the quantities *c(x)* and $Z(x)^T g(x)$ may be regarded as a measure of the error at *x*. The next lemma states that, for a large enough weight, the merit function may also be regarded as a measure of the error.

Lemma 3.4 *Suppose that Assumptions 3.2 hold at* x«. *Then for any \x satisfying (2.23) there exist constants* 73 > 0 *and* 74 > 0, *such that for all x sufficiently near x**

$$\text{TSII* " *.}||^2 \lesssim M^x) \sim M^{x}") \lesssim 74\ [\backslash\backslash Z(xf_9(x)\backslash\backslash^2 + ||c(x)||ij\ . \quad (3.12)$$

Proof. To show the left inequality holds we can write:

$$
\begin{aligned}
*_{„}(*)-*_{„}(*.) &= /(*)+/i||c(z)||_1-/(*,) && (3.13)\\
&= /(*) + X(xfc(x) + |AI||C(X)||I - X(xfc(x)\} - /(x.) && (3.14)\\
&\geq L(x, A.) + (A(x) - \backslash(x,)fc(x) + p\backslash\backslash c(x)\backslash\backslash i - /(x.) && (3.15)\\
&\geq L(x,A.) + |||c(x)||i-/(x.) && (3.16)\\
& && (3.17)
\end{aligned}
$$

where the last inequality follows for all *x* sufficiently near *x. Expanding the last inequality in a Taylor series leads to:**

$$
\begin{aligned}
\phi_\mu(x) - \phi_\mu(x_*) \geq\ & \nabla L(x_*, \lambda_*)^T (x - x_*) + \frac{1}{2}(x - x_*)^T \nabla^2_{xx} L(x_*, \lambda_*)(x - x_*)\\
& + f\ \|c(x)\|_1 + \wedge\|c(x)\|^2 - \wedge||c(x)||^2 + O(\backslash\backslash x - x.||)^3 && (3.18)
\end{aligned}
$$

Now we note that

$$\wedge Mx)f = {}^{U}\text{-}\frac{}{2}\{x - x.)^T A.jg(x - x.) + O(\backslash\backslash x - x.\backslash\backslash)^3. \quad (3.19)$$

In Lemma 4.2 of Byrd and Nocedal (1991) it is shown that if Assumptions 3.2 are satisfied there exist sufficiently large values of *v* such that:

$$\bullet\ |(x - x.)^T (V^2_{xx} L(x_b, A.) + vA.A^*_*)(x - x.) \gtrsim 2_{73}||a; - x.f \quad (3.20)$$

Now since there exists a $K_c > 0$ such that ||c(a;)||i $\lesssim K_c\backslash\backslash x — x_m\backslash\backslash$ we have for ||i — x,|| ≤ *p/(2vK_c):*

$$
\begin{aligned}
\phi_\mu(x) - \phi_\mu(x_*) &\geq 2\gamma_3\|x - x_*\|^2 + \wedge\ \|c(x)\|_1 + O(\|x\ )^3 && (3.21)\\
&\geq 73lk\text{-}ar.ll^2 && (3.22)\\
& && (3.23)
\end{aligned}
$$

for all x sufficiently close to x*. The right inequality follows directly from:

$$
\begin{aligned}
Ms)-</>*(*\bullet) &= /(*) + H|c(x)||i-/(x*) && (3.24)\\
&= L(x, A) - f(x.) + Mk(*)lli \text{ ''} Hxfc(x)\} && (3.25)\\
&\le O(\|x - x4^2) + p\backslash\backslash c(x)h && \mathbf{(3.26)}\\
&\le \gamma_4[\|Z(x)^T{}_9(a:)\|^2 + \|c(x)\|_1] \quad * && (3.27)
\end{aligned}
$$

D

Note that the left inequality in (3.12) implies that for a sufficiently large value of the penalty parameter, the merit function will have a strong local minimizer at x*. We will now use the descent property of Algorithm I to show convergence of the algorithm. However, due to the non-convexity of the problem, the line search could generate a step that decreases the merit function but that takes us away from the neighborhood of x*. To rule this out we make the following assumption.

Assumption 3.3 The line search has the property that, for all large A;, <^((1 — *9)xk* + *Oxk+i)* $\le$ 0/x(#fc) f°r all *6* E [0,1]. In other words, x/t+i is in the connected component of the level set *{x* : $</>_M(x)$ $\le$ *4>p{xk)}* that contains x*.

There is no practical line search algorithm that can guarantee this condition, but it is likely to hold close to x*. Assumption 3.3 is made by Byrd, Nocedal and Yuan (1987) when analyzing the convergence of variable metric methods for unconstrained problems, as well as by Byrd and Nocedal (1991) in the analysis of Coleman-Conn (1984) updates for equality constrained optimization.

Lemma 3.5 *Suppose that the iterates generated by Algorithm I are contained in a convex region D satisfying Assumptions 3.1. If an iterate Xk_Q is sufficiently close to a solution point* x* *that satisfies Assumptions 3.2, and if the weight* $/i\wedge_0$ *is large enough, then the sequence of iterates converges to x*.*

Proof. The proof is virtually identical to the one given in our previous paper. By Assumptions 3.1 (I)-(II) and (1.24) we know that {||Afc||} is bounded. Therefore the procedure (2.42) ensures that the weights /x* are constant, say /ijb = /i for all large fc. Moreover, if an iterate gets sufficiently close to x*, we know by (2.42) and by the continuity of A that (2.23) is satisfied. For such a value of /i, Lemma 3.2 implies that the merit function has a strict local minimizer at x*. Now suppose that once the penalty parameter has settled, and for a given *e* > 0, there is an iterate Xk_0 such that

$$\|x_{k_0} - x_*\| \le \frac{\gamma_3}{\gamma_2\gamma_4\hat{\gamma}_0}\epsilon^2,$$

where 70 is such that $\| \bullet \|_i \le 70\mathrm{II} \bullet \mathrm{II}$ Assumption 3.3 shows that for any $k \ge k_0$, x* is in the connected component of the level set of $x*_0$ that contains Xfc_0, and we can assume that c is small enough that Lemmas 3.3 and 3.4 hold in this level set. Thus since

4>iii^x k)≤ <j>n(^x k_o) for Δ; > /to, and since we can assume that ||£j^<feoll ≤ 1> we have from Lemmas 3.3 and 3.4, for any $k \geq ko$

$$
\begin{aligned}
\|x_k - x_*\| &\leq \gamma_3^{-\frac{1}{2}} (\phi_\mu(x_k) - \phi_\mu(x_*))^{\frac{1}{2}} \\
&\leq \gamma_3^{-\frac{1}{2}} (\phi_\mu(x_{k_0}) - \phi_\mu(x_*))^{\frac{1}{2}} \\
&\leq \left(\frac{\gamma_4}{\gamma_3}\right)^{\frac{1}{2}} \left[\|Z_{k_0}^T g_{k_0}\|^2 + \|c_{k_0}\|_1\right]^{\frac{1}{2}} \\
&\leq (\wedge\ )^{\frac{1}{2}} \left[\|Z_{k_0}^T g_{k_0}\|^2 + \hat{\gamma}_0 \|c_{k_0}\|\right]^{\frac{1}{2}} \\
&\leq \left(\frac{\gamma_2\gamma_4\hat{\gamma}_0}{\gamma_3} \|x_{k_0} - x_*\|\right)^{\frac{1}{2}} \\
&\leq \epsilon.
\end{aligned}
$$

This implies that the whole sequence of iterates remains in a neighborhood of radius e of x+. If e is small enough we conclude by (3.12), by the monotonicity of {(f>n{x_k)} and Theorem 4.2 that the iterates converge to x».

D

3.3. **R-Linear Convergence.**

For the rest of the paper we assume that the iterates generated by Algorithm I converge to x«, which implies that for all large k and some $p > 0$, /x* = /x and

$$»\|c(x)\|\geq \|(xfc(x)\|+pMx)\| \tag{3.28}$$

The analysis that follows depends on how often BFGS updating is applied, and to make this concept precise we define U to be the set of iterates at which BFGS updating takes place,

$$U = \{k : B_M = BFGS(B_k, s_k, y_k)\}, \tag{3.29}$$

and let

$$U_k = UD\ \{1,2, ..,\&\}. \tag{3.30}$$

The number of elements in U_k will be denoted by $\backslash U_k \backslash$. The following result from our previous paper carries over directly to the multiplier-free method.

Theorem 3.6 *Suppose that the iterates* $\{x_k\}$ *generated by Algorithm I converge to a point* x^* *that satisfies Assumptions 3.2. Then for any* k *£U and any* $j \geq k$

$$\|x_j - x_*\| \leq C r^{|U_k|}, \tag{3.31}$$

for some constants $C > 0$ *and* $0 \leq r < 1$.

This result implies that if *{\Uk\/k}* is bounded away from zero, then Algorithm I is R-lineaxly convergent. However, BFGS updating could take place only a finite number of times, in which case this ratio would converge to zero. It is also possible for BFGS updating to take place an infinite number of times, but every time less often, in such a way that $\backslash U_k \backslash /k$ —¥ 0. We therefore need to examine the iteration more closely.

We make use of the matrix function *ip* defined by

$$\psi(B) = tr\{B) - \ln(\mathrm{cfct}(B)), \tag{3.32}$$

where *tr* denotes the trace, and *det* the determinant. It can be shown that

$$\mathrm{lncond}(B)<V>(£), \tag{3.33}$$

for any positive definite matrix *B* (Byrd and Nocedal (1989)). We also make use of the weighted quantities

$$\tilde{V}k = G7^{1/2}y_k, \qquad \tilde{s}_k = G^lJ^2s_k, \tag{3.34}$$

$$\tilde{B}_k = G;^{1/2}B_{fc}G;^{1/2}, \tag{3.35}$$

$$\cos\tilde{\theta}_k = \frac{\tilde{s}_k^T\tilde{B}_k\tilde{s}_k}{\|£*«*\|\|\|**\|}, \tag{3.36}$$

and

$$\tilde{q}_k = 2g\wedge_{\tilde{s}_k s_k} \tag{3.37}$$

One can show (see eq. (3.22) of Byrd and Nocedal (1989)) that if B_k is updated by the BFGS formula then

$$\begin{aligned}\psi(\tilde{B}_{k+1}) &= \psi(\tilde{B}_k) + \frac{\|\tilde{y}_k\|^2}{\tilde{y}_k^T\tilde{s}_k} - 1 - \ln\frac{\tilde{y}_k^T\tilde{s}_k}{\tilde{s}_k^T\tilde{s}_k} + \ln\cos^2\tilde{\theta}_k \\ &+ \left[1 - \frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k} + \ln\frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k}\right].\end{aligned} \tag{3.38}$$

This expression characterizes the behavior of the BFGS matrices B_{ky} and will be crucial to the analysis of this section. However before we can make use of this relation we need to consider the accuracy of the correction terms. We begin by showing that when finite differences axe used to estimate w_k and TU\, these axe accurate to second order.

Lemma 3.7 *// at the iterate x_k, the corrections w_k and $\overline{w_k}$ are computed by the finite difference formulae (2.1)-(2.2), and if x_k is sufficiently close to a solution point* z* *that satisfies Assumptions 3.2, then*

$$«»* = O(\mathrm{lbvll}), \tag{3-39}$$

$$\mathrm{IK} - Z,^{r}W.y_{fe}p_Y\| = O\{a_k\backslash\backslash p_Y\backslash\backslash) \tag{3.40}$$

and

$$\|\overline{w}_k - \alpha_k Z^TW_*Y_kp_Y\| = O(\sigma_k\|p_Y|\backslash). \tag{3.41}$$

Proof. The proof requires only a minor modification of the same property proved in the previous paper. Recalling that VL(z, A) = $g(x)$ + A(x)A, we have from (2.1) that

$$\begin{aligned} w_k &= Z(x_k + Y_k\bar{p}_Y)^T g\{x_k + Y_k p_Y) - Z(x_k)^T g(x_k) \\ &= Z(x_k + Y_k p_Y)^T VL(x_k + Y_k p_Y, A,) - Z(x_k)^T VL(x_k, A,) \\ &= (Z(x_k + Y_k p_Y) - Z(x_k))^T VL(x_k + Y_k p_Y, \backslash *) \\ &\quad + Z_k^T \left[\int_0^1 V^2_{xx} L\{x_k + rY_k p_Y, A,) rfr \right] Y_k p_Y \\ &\equiv Z_k^T \overline{W}_k Y_k p_Y + (Z(x_k + npy) - Z(x^*))^r VL(a^* + Y_k p_Y, A,) \\ &= Z_k^T \overline{W}_k Y_k p_Y + O(\sigma_k)\|p_Y\| \end{aligned} \quad (3.42)$$

The above result follows for x_k in the neighborhood of £* where (3.6)-(3.9) hold because:

$$VL(x_k + Y_k p_Y, A.) = O(\|x - x_m\backslash\backslash) + O(|b_Y\|) = O(a_{fc}) \quad (3.43)$$

where a_k is defined by (1.29). Also a simple computation shows that

$$[ZlW_k - Z?W.]Y_{kPY} = \mathbf{OVibllPvll).)} \quad \mathbf{(3.44)}$$

Using these facts in (3.42) yields the desired result (3.40). To prove (3.41), we only note that $a_k \leq 1$, and reason in the same manner. D

Next we show that the condition number of the matrices B_k is bounded, and that at the iterates U at which BFGS updating takes place the matrices B_k are accurate approximations of the reduced Hessian of the Lagrangian.

Theorem 3.8 *Suppose that the iterates $\{x_k\}$ generated by Algorithm I converge to a solution point x^* that satisfies Assumptions 3.2. Then* {||B^||} *and* $\{\backslash\backslash B^{\wedge l}\backslash\backslash\}$ *are bounded, and for allkeU*

$$\|(B_k - Z^\wedge \quad Z_*)p_Z\| = o(\|d_k\|). \quad (3.45)$$

Proof. Again, the proof follows along the same lines as the one in our previous paper, but with slight modification. Consider only iterates k for which BFGS updating of Bk takes place. We have from (2.50), (2.48), (2.46), (2.12) and (2.49)

$$\begin{aligned} y_k &= Zj_{+1} g_{k+1} - Zlg_k - \overline{w}_k \\ &= Z_{k+1}^T \nabla L(x_{k+1}, X,) - Z][VL(x_k, X,) - \overline{w}_k \\ &= (Z_{k+1} - Z_k f VL(x_{k+1}, A.) + ZftVLfo{+}i, A.) - VL(x_k, A.)) - \overline{w}_k \\ &= (Z_{k+1} - Z_k)^T VL\{x_{k+u} A,) + [zj\, jf_0^1 V^2_{xx} L(x_k + Ta_k d_k, A,) rfr]\, a_k d_k - \overline{w}_k \\ &= ct_k Zl\tilde{W}_k\{Z_{kPz} + Y_k p_Y) - \overline{w_k} + O(<7_{fc})(\|a_{fc}\| + a_k\|p_Y\|) \\ &= Z\bar{l}W_k Z_k s_k + a_k\{Zl\tilde{W}_k - ZT\backslash V.)Y_k p_Y + (a_k ZjW.Y_k p_Y - \overline{w}_k) \\ &\quad + O(a_k)(\backslash\backslash s_k\backslash\backslash + a_k\backslash\backslash p_Y\backslash\backslash). \end{aligned} \quad (3.46)'$$

Since $\bar{w}_k$ can be computed by Broyden's method or by finite differences, we consider these two cases separately.

Part I. We first assume that $\bar{w}_k$ is determined by Broyden's method. A simple computation shows that $\|Z_*^T[\tilde{W}_k - Z_*^T W_*]\| = O(\sigma_k)$, and from (2.10) we have that $\bar{w}_k = O(\|p_Y\|/\gamma_k)$. Using this and Assumptions 3.2 in (3.46) we have

$$\begin{aligned} y_k &= Z_k^T \tilde{W}_k Z_k s_k + (\sigma_k + 1 + 1/\gamma_k)O(\alpha_k\|p_Y\|) + O(\sigma_k)\|s_k\| \\ &= (Z_*^T \tilde{W}_k Z_k - G_*)s_k + G_* s_k + (\sigma_k + 1 + 1/\gamma_k)O(\alpha_k\|p_Y\|) + O(\sigma_k)\|s_k\|. \end{aligned} \tag{3.47}$$

Recalling (3.34) and noting that $\tilde{y}_k^T \tilde{s}_k = y_k^T s_k$ we have

$$\tilde{y}_k^T \tilde{s}_k = s_k^T(Z_*^T \tilde{W}_k Z_k - G_*)s_k + \|\tilde{s}_k\|^2 + (\sigma_k + 1 + 1/\gamma_k)O(\alpha_k\|p_Y\|)\|\tilde{s}_k\| + O(\sigma_k)\|s_k\|^2,$$

since $\|\tilde{s}_k\|$ and $\|s_k\|$ are of the same order. Therefore

$$\begin{aligned} \frac{\tilde{y}_k^T \tilde{s}_k}{\|\tilde{s}_k\|^2} &= 1 + \frac{s_k^T(Z_*^T \tilde{W}_k Z_k - G_*)s_k}{\|\tilde{s}_k\|^2} \\ &\quad + (\sigma_k + 1 + 1/\gamma_k)O\left(\frac{\|\alpha_k p_Y\|}{\|\tilde{s}_k\|}\right) + O(\sigma_k) \\ &= 1 + O(\sigma_k) + (\sigma_k + 1 + 1/\gamma_k)O\left(\frac{\|\alpha_k p_Y\|}{\|\tilde{s}_k\|}\right). \end{aligned} \tag{3.48}$$

Similarly from (3.47) and (3.34) we have

$$\begin{aligned} \tilde{y}_k^T \tilde{y}_k \le\; & \|(Z_k^T \tilde{W}_k Z_k - G_*)s_k\|^2 \|G_*^{-1}\| \\ & + 2(1 + O(\sigma_k))\|(Z_*^T \tilde{W}_k Z_k - G_*)s_k\| \, \|G_*^{-1/2}\| \, \|\tilde{s}_k\| + (1 + O(\sigma_k))^2\|\tilde{s}_k\|^2 \\ & + 2(\sigma_k + 1 + 1/\gamma_k)O(\|\alpha_k p_Y\|)\|G_*^{-1/2}\| \left((1 + O(\sigma_k))\|\tilde{s}_k\| + \|(Z_*^T \tilde{W}_k Z_k - G_*)s_k\|\|G_*^{-1/2}\|\right) \\ & + (\sigma_k + 1 + 1/\gamma_k)^2 O(\|\alpha_k p_Y\|)^2, \end{aligned} \tag{3.49}$$

and thus

$$\begin{aligned} \frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} \le\; & 1 + O(\sigma_k) + (\sigma_k + 1 + 1/\gamma_k)(1 + \sigma_k)O\left(\frac{\|\alpha_k p_Y\|}{\|\tilde{s}_k\|}\right) \\ & + (\sigma_k + 1 + 1/\gamma_k)^2 O\left(\frac{\|\alpha_k p_Y\|^2}{\|\tilde{s}_k\|^2}\right). \end{aligned} \tag{3.50}$$

At this point we invoke the update criterion, and note from (2.14) that if BFGS updating of B_k takes place at iteration k, then $\|\alpha_k p_Y\| \le \gamma_k^2\|\tilde{s}_k\|$ where $\{\gamma_k\}$ is summable. Using this, the assumption that σ_k converges to zero, and (3.48) we see that for large k

$$\frac{\tilde{y}_k^T \tilde{s}_k}{\|\tilde{s}_k\|^2} = 1 + O(\sigma_k + \gamma_k), \tag{3.51}$$

and using (3.50)

$$\frac{\|\tilde y_k\|^2}{\|\tilde s_k\|^2} = 1 + O(\sigma_k + \gamma_k).$$

Therefore

$$\frac{\|\tilde y_k\|^2}{\tilde y_k^T \tilde s_k} = \frac{\|\tilde y_k\|^2}{\|\tilde s_k\|^2}\frac{\|\tilde s_k\|^2}{\tilde y_k^T \tilde s_k} = 1 + O(\sigma_k + \gamma_k). \tag{3.52}$$

We now consider $\psi(\tilde B_{k+1})$ given by (3.38). A simple expansion shows that for large k, $\ln(1 + O(\sigma_k + \gamma_k)) = O(\sigma_k + \gamma_k)$. Using this, (3.51) and (3.52) we have

$$\psi(\tilde B_{k+1}) = \psi(\tilde B_k) + O(\sigma_k + \gamma_k) + \ln\cos^2\tilde\theta_k + \left[1 - \frac{\tilde q_k}{\cos^2\tilde\theta_k} + \ln\frac{\tilde q_k}{\cos^2\tilde\theta_k}\right]. \tag{3.53}$$

Note that for $x \geq 0$ the function $1 - x + \ln x$ is non-positive, implying that the term in square brackets is non-positive, and that $\ln\cos^2\tilde\theta_k$ is also non-positive. We can therefore delete these terms to obtain

$$\psi(\tilde B_{k+1}) \leq \psi(\tilde B_k) + O(\sigma_k + \gamma_k). \tag{3.54}$$

Before proceeding further we show that a similar expression holds when finite differences are used.

Part II. Let us now consider the iterates k for which updating takes place and for which $\bar w_k$ is computed by finite differences. In this case (2.15) holds. Again we begin by considering (3.46),

$$y_k = Z_k^T W_k Z_k s_k + \alpha_k(Z_k^T W_k - Z_*^T W_*)Y_k p_Y + (\alpha_k Z_*^T W_* Y_k p_Y - \bar w_k) + O(\sigma_k)(\|s_k\| + \alpha_k\|p_Y\|).$$

Using (3.41) the second and third terms are of order $\sigma_k(\alpha_k\|p_Y\|)$. Thus

$$\begin{aligned} y_k &= Z_k^T \tilde W_k Z_k s_k + O(\sigma_k)(\|s_k\| + \alpha_k\|p_Y\|) \\ &= (Z_k^T \tilde W_k Z_k - G_*)s_k + G_* s_k + O(\sigma_k)(\|s_k\| + \alpha_k\|p_Y\|). \end{aligned} \tag{3.55}$$

Noting once more that $\tilde y_k^T \tilde s_k = y_k^T s_k$ and recalling the definition (3.34) we have

$$\tilde y_k^T \tilde s_k = \tilde s_k^T (Z_k^T \tilde W_k Z_k - G_*)\tilde s_k + \|\tilde s_k\|^2 + O(\sigma_k)(\|\tilde s_k\|^2 + \alpha_k\|p_Y\|\|\tilde s_k\|),$$

since $\|\tilde s_k\|$ and $\|s_k\|$ are of the same order. Therefore

$$\begin{aligned} \frac{\tilde y_k^T \tilde s_k}{\|\tilde s_k\|^2} &= 1 + \frac{\tilde s_k^T (Z_k^T \tilde W_k Z_k - G_*)\tilde s_k}{\|\tilde s_k\|^2} + O(\sigma_k)\left(1 + \frac{\|\alpha_k p_Y\|}{\|\tilde s_k\|}\right) \\ &= 1 + O(\sigma_k) + O\left(\sigma_k \frac{\|\alpha_k p_Y\|}{\|\tilde s_k\|}\right). \end{aligned} \tag{3.56}$$

Similarly from (3.55) and (3.34) we have

$$
\begin{aligned}
\tilde{y}_k^T \tilde{y}_k \le\ & \|(Z_k^T \tilde{W}_k Z_k - G_*) s_k\|^2 \|G_*^{-1}\| \\
& + 2(1 + O(\alpha_k)) \|(Z_k^T \tilde{W}_k Z_k - G_*) s_k\| \, \|G_*^{-1/2}\| \, \|p_*\| + (1 + O(\alpha_k)) \|\tilde{s}_k\|^2 \\
& + \sigma_k O\left(\|\alpha_k p_Y\| \|G_*^{-\frac{1}{2}}\| \left[(1 + O(\alpha_k)) \|\tilde{s}_k\| + \|(Z_k^T \tilde{W}_k Z_k - G_*) s_k\| \|G_*^{-1/2}\| \right] \right) \\
& + 4O(\|\alpha_k p_Y\|)^2,
\end{aligned}
$$

and thus

$$
\frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} \le 1 + O(\alpha_k) + \alpha_k O\left(\frac{\|p_Y\|}{\|s_k\|} \right) + \sigma_k O\left(\frac{\|\alpha_k p_Y\|^2}{\|s_k\|^2} \right). \qquad (3.57)
$$

The rest of the proof is identical to the one in our previous paper. We note from (2.15) that if BFGS updating of B_k takes place at iteration k, then $\|p_Y\| \le \gamma_d \|p_Z\| / \sigma_k^{1/2}$. Using this, (3.56) and the fact that G_k converges to zero, we see that for large k

$$
\frac{\tilde{y}_k^T \tilde{s}_k}{\|\tilde{s}_k\|^2} = 1 + O(\sigma_k^{1/2}),
$$

and using (3.57)

$$
\frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} = 1 + O(\sigma_k^{1/2}).
$$

Therefore

$$
\frac{(\tilde{y}_k^T \tilde{s}_k)^2}{\|\tilde{y}_k\|^2 \|\tilde{s}_k\|^2} = 1 + O(\sigma_k^{1/2}). \qquad (3.58)
$$

We now consider $\psi(\tilde{B}_{k+1})$ given by (3.38). Noting that $\ln(1 + O(\alpha_k^{1/2})) = O(\alpha_k^{1/2})$ for all large k, we see that if updating takes place at iteration k

$$
\psi(\tilde{B}_{k+1}) = \psi(\tilde{B}_k) + O(\alpha_k^{1/2}) + \ln \cos^2 \tilde{\theta}_k + \left[1 - \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} + \ln \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} \right]. \qquad (3.59)
$$

Since both $\ln \cos^2 \tilde{\theta}_k$ as well as the term inside the square brackets are non-positive, we can delete them to obtain

$$
\psi(\tilde{B}_{k+1}) \le \psi(\tilde{B}_k) + O(\alpha_k^{1/2}). \qquad (3.60)
$$

We now combine the results of Parts I and II of this proof. Let us subdivide the set of iterates U for which BFGS updating takes place into two subsets: U' corresponds to the iterates in which $\overline{W}_k$ is computed by Broyden's method, and U'' to the iterates in which finite differences are used. We also define $U'_k = U' \cap \{1, 2, \ldots k\}$ and $U''_k = U'' \cap \{1, 2, \ldots k\}$.

Summing over the set of iterates in U''_k, using (3.54) and (3.60), and noting that $B_{j+1} = B_j$ for $j \notin U_k$, we have

$$
\psi(\tilde{B}_{k+1}) \le \psi(\tilde{B}_1) + C_1 \sum_{j \in U''_k} \alpha_j^{1/2} + C_2 \sum_{j \in U'_k} \sigma_j + C_3 \sum_{j \in U'_k} \ldots \qquad (3.61)
$$

for some constants $C_U C_2, C_3$. By (3.31) and since $|U_j''| \leq |U_j|$,

$$\sum_{j\in U''} a_j^{1/2} \leq \sum_{j\in U''} C^{1/2} r^{|U_j|/2}$$

$$\leq \sum_{j\in U''} C^{1/2} r^{|U_j''|/2}$$

$$= \sum_{i=1}^{|U''|} C^{1/2} r^{i/2}$$

$$< \infty.$$

Similarly

$$\sum_{j\in U'} a_j < \infty,$$

and since {7*} is summable we conclude from (3.61) that *{xp(B̃k)}* is bounded above. By (3.32) *tl>(B̃k)* = SJLiCt"- ln^t)> where Zj are the eigenvalues of ĩ?*, and it is easy to see that this implies that both Hi?*II and HB^[1]!! are bounded.

To prove (3.45), we sum relations (3.53) and (3.59), recalling that a*, 7* and $o^{1/2}$ are summable, to obtain

$$\psi(\tilde{B}_{k+1}) \leq C + \sum_{j\in U_k} \left(\ln \cos^2 \tilde{\theta}_k + \left[1 - \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} + \ln \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} \right] \right),$$

for some constant *C.* Since $\psi(\tilde{B}_{k+1}) > 0$, and since both $\ln \cos^2 \tilde{\theta}_k$ and the term inside the square brackets are non-positive we see that

$$\lim_{\substack{k\to\infty \\ k\in U}} \ln \cos^2 \tilde{\theta}_k = 0,$$

and

$$\lim_{\substack{k\to\infty \\ k\in U}} \left[1 - \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} + \ln \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} \right] \to 0.$$

Now, for $x \geq 0$ the function $1 - x + \ln x$ is concave and has its unique maximizer at $x = 1$. Therefore the relations above imply that

$$\lim_{\substack{k\to\infty \\ k\in U}} \cos \tilde{\theta}_k = \lim_{\substack{k\to\infty \\ k\in U}} \tilde{q}_k = 1. \qquad (3.62)$$

Now from (3.36)-(3.37)

$$\frac{\|G_*^{-1/2}(B_k - G_*) p_k\|^2}{\|G_*^{1/2} p_k\|^2} = \frac{\|(\tilde{B}_k - I)\tilde{s}_k\|^2}{\|\tilde{s}_k\|^2}$$

$$= \frac{\|\tilde{B}_k \tilde{s}_k\|^2 - 2\tilde{s}_k^T \tilde{B}_k \tilde{s}_k + \tilde{s}_k^T \tilde{s}_k}{\tilde{s}_k^T \tilde{s}_k}$$

$$= \frac{\tilde{q}_k^2}{\cos^2 \tilde{\theta}_k} - 2\tilde{q}_k + 1.$$

Convergence Analysis for a Multiplier-Free Reduced Hessian Method

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CONVERGENCE ANALYSIS FOR A MULTIPLIER FREE REDUCED HESSIAN METHOD

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We propose a quasi-Newton algorithm for solving optimization problems with nonlinear equality constraints. It is designed for problems with few degrees of freedom and does not require the calculation of Lagrange multipliers. It can also be extended to large-scale systems through the use of sparse matrix factorizations. The algorithm has the same superlinear and global properties as the reduced Hessian method developed in our previous paper (Biegler, Nocedal and Schmid, 1995). This report directly reworks the theory presented in that paper to consider the multiplier free case.

1. Introduction.

We consider the nonlinear optimization problem

$$\min_{x\in\mathbf{R}^n} f(x) \tag{1.1}$$

$$\text{subject to } \; c(x) = 0, \tag{1.2}$$

where $f : \mathbf{R}^n \to \mathbf{R}$ and $c : \mathbf{R}^n \to \mathbf{R}^m$ are smooth functions. We assume that the first derivatives of f and c are available, but our algorithm does not require second derivatives. The successive quadratic programming (SQP) method for solving (1.1)-(1.2) generates, at an iterate x_k, a search direction d_k by solving

$$\min_{d\in\mathbf{R}^n} \; g(x_k)^T d + \tfrac{1}{2} d^T W(x_k) d \tag{1.3}$$

$$\text{subject to } \; c(x_k) + A(x_k)^T d = 0, \tag{1.4}$$

where g denotes the gradient of f, W denotes the Hessian of the Lagrangian function $L(x, \lambda) = f(x) + \lambda^T c(x)$, and A denotes the n x m matrix of constraint gradients

$$A(x) = [\nabla c_1(x), ..., \nabla c_m(x)]. \tag{1.5}$$

A new iterate is then computed as

$$x_k+\backslash = x_k + a_k d_k, \tag{1.6}$$

where a_k is a steplength parameter chosen so as to reduce the value of the merit function. In this study we will use the $t\backslash$ merit function

$$\wedge(x) = /(x) + _M||c(x)||_1, \tag{1.7}$$

where /i is a penalty parameter; see for example Conn (1973), Han (1977) or Fletcher (1987). This penalty parameter is normally based on Lagrange multiplier values or their estimates but here we consider a simpler measure that does not require Lagrange multiplier estimates, but still maintains descent properties for *(fi^x)*.

The solution of the quadratic program (1.3)-(1.4) can be written in a simple form if we choose a suitable basis of R^n to represent the search direction d_k. For this purpose, we introduce a nonsingular matrix of dimension n, which we write as

$$[Y_k Z_k], \tag{1.8}$$

where Y_k *e* $R^{n\times m}$ and Z_k € R«^{x}(^{n}-^{m}), and assume that

$$AlZ_k = 0. \tag{1.9}$$

(From now on we abbreviate $A(x_k)$ as A_k, $g(x_k)$ as g_k, etc.) Thus Z_k is a basis for the tangent space of the constraints. We can now express d_k, the solution to (1.3)-(1.4), as

$$d_k = Y_k p_Y + Z_{kPz}, \tag{1.10}$$

for some vectors p_Y € R^m and p_z € $R^n{\sim}^m$. Due to (1.9) the linear constraints (1.4) become

$$c_k + AlY_k p_Y = 0. \tag{1.11}$$

If we assume that *Ak* has full column rank then the nonsingularity of *[Yk Zk]* and equation (1.9) imply that the matrix $A^\wedge Y_k$ is nonsingular, so that p_Y is determined by (1.11):

$$p_Y = -[A_k^T Y_k]^{-1} c_k. \tag{1.12}$$

Substituting this in (1.10) we have

$$d_k = -Y_k[AlY_h]^{-1}Ck + Z_{kPz}. \tag{1.13}$$

The SQP sub-problem can now be expressed exclusively in terms of the variables p_z. Substituting (1.10) into (1.3), considering $Y_k p_Y$ as constant, and ignoring constant terms, we obtain the unconstrained quadratic problem

$$\min_{p_Z \in \mathbf{R}^{n-m}} (Z_k^T g_k + Z_k^T W_k Y_k p_Y)^T p_Z + \backslash\ p_Z{}^T(Z_k^T W_k Z_k)p_Z. \quad 1 \quad 4 \quad)$$

Assuming that $Z\%W_kZ_k$ is positive definite, the solution of (1.14) is

$$p_z = -(Zl\ W_k[Z_kZ)^{-1}\ g_k + ZlW_kY_kp_Y). \qquad (1.15)$$

This determines the search direction of the SQP method.

In our previous paper (Biegler, Nocedal and Schmid, 1995) the cross term $[Z^T_k W_k Y_k \backslash p_Y$ is approximated by a vector it;*,

$$[ZlW_kY_k]p_Y{*}w_k, \qquad (1.16)$$

without computing the matrix $Z\%W_kY_k$. This allows the rate of convergence of the algorithm to be 1-step Q-superlinear, as opposed to the 2-step superlinear rate for methods that ignore the cross term (Byrd (1985) and Yuan (1985)). The null space step (1.15) of our algorithm will be given by

$$p_z = -\{ZlW_kZ_k)^{-1}[Zlg_k + (_kw_k), \qquad (1.17)$$

where $0 < (_k \leq 1$ is a damping factor described in our previous paper.

Here the cross term is approximated either by a finite difference estimate along Y_kp_Y or by a quasi-Newton method in which the rectangular matrix $Z\hat{}W_k$ is approximated by a matrix S_k, using Broyden's method. We then obtain w_k by multiplying this matrix by Y_kp_Y, i.e.,

$$w_k = S_kY_kp_Y.$$

In this study, we update $S_k+\backslash$ so that it satisfies the following secant relation:

$$S_k+i(x_M - x_k) = Zl+_{l9}(x_k+i) - Zlg\{x_k). \qquad (1.18)$$

Let us now consider how to approximate the reduced Hessian matrix $Z\hat{}W_kZ_k$. Prom (1.6), (1.10) and (1,18) we obtain

$$[S_k+iZ_k]a_kp_z = -a_kS_k+i(Y_kp_Y) + Z\hat{}gixk+i) - Zlg(x_k).$$

Since $S_k+\backslash$ approximates Z^TW, this suggests the following secant equation for 27&+1, the quasi-Newton approximation to the reduced Hessian Z^TWZ:

$$B_{k+1}s_k = y_k, \qquad (1.19)$$

where s_k and y_k are defined by $s_k = a_kp_z$, and

$$Vk = ZZ+_{l9}(x_k+0 - Zlg\{x_k) - \overline{w}_k, \qquad (1.20)$$

with

$$W_k = a_kS_M(Y_kp_Y). \qquad (1.21)$$

We will update B_k by the BFGS formula (cf. Fletcher (1987))

$$B_{k+1} = B_k - \frac{B_ks_ks_k^TB_k}{s_k^TB_ks_k} + \frac{y_ky_k^T}{y_k^Ts_k}, \qquad (L22)$$

provided $s_k^T y_k$ is sufficiently positive. As a result, the null space step is computed from:

$$B_k p_Z = -(Z_k^T g_k + \omega_k) \quad (1.23)$$

Note as in our previous paper, that two correction terms, w_k and $\bar{w}_k$ are applied. The first term, w_k, is used in the null space step (1.23) and makes Use of the matrix S_k. The second term, $\bar{w}_k$ is used in (1.20) for the BFGS update of B_k and is computed using the new Broyden matrix S_{k+1}, and takes into account the steplength α_k. We will see below that it is useful to incorporate the most recent information in $\bar{w}_k$.

Finally, as noted by Orozco (1993), an interesting relationship in the definition of basis representations and Lagrange multipliers occurs for a particular choice of Z and Y. If we define the Lagrange multiplier estimates by:

$$\lambda(x) = -[Y(x)^T A(x)]^{-T} Y(x)^T g(x). \quad (1.24)$$

and partition x into m basic or dependent variables (which without loss of generality are assumed to be the first m variables) and $n - m$ nonbasic or control variables, we induce the partition

$$A(x)^T = [C(x) N(x)], \quad (1.25)$$

where the $m \times m$ basis matrix $C(x)$ is assumed to be nonsingular. We now define $Z(x)$ and $Y(x)$ to be

$$Z(x) = \begin{bmatrix} -C(x)^{-1}N(x) \\ I \end{bmatrix}, \quad Y(x) = \begin{bmatrix} I \\ 0 \end{bmatrix}. \quad (1.26)$$

This choice is particularly advantageous when $A(x)$ is large and sparse, because a sparse LU decomposition of $C(x)$ can often be computed efficiently, and this approach will be considerably less expensive than a QR factorization of $A(x)$. It is also straightforward to show that for any points $\bar{x}$, $\hat{x}$ for which $C(\bar{x})$, $C(\hat{x})$ are nonsingular, we have

$$Z(\hat{x})^T \nabla L(\bar{x}, \lambda(\bar{x})) = Z(\bar{x})^T g(\bar{x}) \quad (1.27)$$

This allows us to make the following equivalence in the calculation of γ_k.

$$\begin{aligned} y_k &= Z_{k+1}^T g(x_{k+1}) - Z_k^T g(x_k) - \bar{w}_k \\ &= Z_k^T \nabla L(x_{k+1}, \lambda_{k+1}) - Z_k^T g(x_k) - \bar{w}_k \end{aligned} \quad (1.28)$$

when (1.26) is chosen for Y and Z.

In the next section we discuss the revised reduced Hessian algorithm in detail. In particular, we briefly describe the calculation of the correction terms w_k and $\bar{w}_k$, the conditions under which BFGS updating takes place, the choice of the damping parameter ζ_k, and the procedure for updating the weight μ_k in the merit function. Most of these steps are identical to the ones in our previous paper. Section 3 presents an analysis of the local behavior of the algorithm, shows that the rate of convergence is at least R-linear and summarizes the properties related to superlinear convergence. Numerical results and extensions to consider variable bounds are described in a companion paper (Biegler, Schmid and Ternet, 1995).

Regarding our notation, throughout the paper the vectors p_Y and p_z are computed at Zfc, and could be denoted by p_Y^ and p_z^^{k}\ but we will normally omit the superscript for simplicity. The symbol || • || denotes the *I2* vector norm or the corresponding induced matrix norm. When using the *l*\ or /<» norms we will indicate it explicitly by writing II • 111 **or** || • Hoc. A solution of problem (1.1) is denoted by x*, and we define

$$e_k = x_k - x+ \quad \text{and} \quad a_k = \mathbf{max\{||e*||,}\ ||e*+i||\}. \tag{1.29}$$

2. Details of the Multiplier-Free Algorithm

In this section we consider[1] how to calculate approximations w_k and $\overline{w}_k$ to *(Z%W_kY_k)p_Y* to be used in the determination of the search direction p_z and in updating 2?*, respectively. We also discuss when to skip the BFGS update of the reduced Hessian approximation, as well as the selection of the damping factor *Ck* and the penalty parameter /i&.

To approximate to $(Z^TWY)p_Y$ we propose two approaches that have slight modifications to those proposed in our earlier paper. First, we consider a finite difference approximation to *Z][*W_k along the direction Y_kp_Y. The second approach defines w_k and $\overline{w}_k$ in terms of a Broyden approximation to *Z%*W_k, as discussed in §1, and requires no additional function or gradient evaluations. Our algorithm will normally use this second approach, although it is sometimes necessary to use finite differences.

2.1. Calculating w_k and $\overline{w}_k$ Through Finite Differences.

We first calculate the range space step p_Y at x_k through equation (1.12). Next we compute the reduced gradient of the Lagrangian at $x_k + Y_kp_Y$ and define

$$w_k = Z(x_k + Y_kp_Yfg(x_k + Y_kp_Y) - Zlg_k. \tag{2.1}$$

After the step to the new iterate x_k+\ has been taken, we define

$$\overline{w}_k = a_kw_k \tag{2.2}$$

which requires a new evaluation of gradients if a_k ^ 1. These correction terms are substituted for the ones used in our previous paper:

$$w_k = Zl[VL\{x_k + \mathbf{Y}_{kPYy}\, X_k) - VL(x_k,\backslash_k)]. \tag{2.3}$$

$$\overline{w}_k = Zl\backslash VL\{x_k + a_kY_kp_Y,\ X_M) - VL\{x_k,\ A*_{+1})] \tag{2.4}$$

2.2. Using Broyden's Method to Compute w_k and $\overline{w}_k$.

We can approximate the rectangular matrix *Z^*W_k by a matrix 5* updated by Broyden's method, and then compute w_k and $\overline{w}_k$ by post-multiplying this matrix by Y_kp_Y

or by a multiple of this vector. As discussed in §1 it is reasonable to impose the secant equation (1.18) on this Broyden approximation, which can therefore be updated by the formula (cf. Fletcher (1987))

$$S_W \wedge g_{fc} + \frac{(fe" \, i \, ! \, ft)}{{}^{s}k^{s}k} \wedge \tag{2.5}$$

where

$$\bar{V}k = Zjf_{+}i0(s^*+i) - Zlg(x_k) \tag{2.6}$$
$$Sk = Zifc{+}i - x_k. \tag{2.7}$$

thus, defining

$$w_k = S_k Y_k p_Y \quad \text{and} \quad \overline{w}_k = a_k S_k + i Y_k p_Y. \tag{2.8}$$

As in our previous paper, we apply a safeguard on these updates to make sure that w_k and $\overline{w}_k$ remain bounded. At the beginning of the algorithm we choose a positive constant T and define

$$w_k := \begin{cases} w_k & \text{if } \|w_k\| \le \frac{\Gamma}{\|p_Y\|^{1/2}} \|p_Y\| \\ w_k \frac{\Gamma \|p_Y\|^{1/2}}{\|w_k\|} & \text{otherwise.} \end{cases} \tag{2.9}$$

On the other hand, the correction $\overline{w}_k$ will be safeguarded by choosing a sequence of positive numbers {7*} such that E-g1^ < 00, and set

$$\overline{w}_k \quad \begin{cases} \overline{w}_k & \text{if } \|\overline{w}_k\| \le \alpha_k \|p_Y\| / \gamma_k \\ \overline{w}_k \frac{\alpha_k \|p_Y\|}{\gamma_k \|\overline{w}_k\|} & \text{otherwise.} \end{cases} \tag{2.10}$$

As the iterates converge to the solution, p_Y —• 0, we see from (2.8) and from the boundedness of Y_k that these safeguards allow the Broyden updates S_k to become unbounded, but in a controlled manner. In our previous paper, it was shown that these Broyden updates S_k do, in fact, remain bounded, so that the safeguards become inactive asymptotically.

2.3. Update Criterion.

It is well known that the BFGS update (1.22) is well defined only if the curvature condition $s^\wedge y_k > 0$ is satisfied. This condition can always be enforced in the unconstrained case by performing an appropriate line search; see for example Fletcher (1987). However when constraints are present the curvature condition $s\%y_k > 0$ can be difficult to obtain, even near the solution.

To show this we first note from (1.20), (1.10) and from the Mean Value Theorem that

$$\begin{aligned} y_k &= Z\% + xgfc{+}i \sim Z_k^T g_k - \overline{w}_k \\ &= Z_{k+1}^T \nabla L(x_{k+1}, \lambda_*) - Z_k^T \nabla L(x_k, \lambda_*) - \overline{w}_k \\ &= Zl \left[\int^1 V^2_{xx} L\{x_k + r a_k d_k, \backslash *) dr \right] a_k d_k + (Z_{fc+}i - Z_k)^T VL(x_k+_u K) - \overline{w}_k \\ &\equiv Zl\tilde{W}_k a_k d_k + (Z^*_{+}i - Zib)^r VL(xfc_{+}i, A^*) - \overline{w}_k \\ &= Z_j' F \tilde{W}_k Z_k s_k + O(a \wedge \|s_k\| + \alpha_k \|p_Y\|) + \alpha_k Z_k^T \tilde{W}_k Y_k p_Y - \overline{w}_k, \end{aligned} \tag{2.11}$$

where we have defined

$$Z_k^T \tilde{W}_k = Zl \int_{Jo}^{1} V^2_{xx} L\{x_k + Ta_k d_k, X.)dr. \quad \textbf{(2.12)}$$

Thus

$$sly_k = s^T_k\{Zl\tilde{W}_k Z_k)s_k + O(a_k)\|_{Sk}f + [a_k sj\,(ZjW_k\tilde{Y}_k)p_Y - \#57^*] + O(o_k)\|a_k\|\ \|py\,\|. \quad (2\text{-}13)$$

Near the solution, the two O(a&) terms will vanish, while the first term on the right hand side will be positive since *Z^W^Zk* can be assumed positive definite. Nevertheless the bracketed terms in (2.13) are of uncertain sign and can make *s^yk* negative. To avoid this problem and also ensure that the quasi-Newton approximation remains boimded, we apply the same updating criterion developed in our previous paper.

Update Criterion I.

Choose a constant $y_{\{d}$ > 0 *and a sequence of positive numbers {jk} such that* Ej^^fc < oo *(this is the same sequence* {7*} *that was used in (2.10)).*

- *IfWk is computed by Broyden's method, and if both s^yk* > 0 *and*

$$\mathbf{Ibvll \le 7^{*2}IM} \quad \textbf{(2.14)}$$

hold at iteration k, then update the matrix Bk by means of the BFGS formula (1.22) with Sk and y* *given by (1.20). Otherwise, set* $B_{k+1} = B_k$.

- *// Wk is computed by finite differences, and if both s£yk* > 0 *and*

$$\|p_Y\| \le \gamma_{fd}\|p_Z\|/\sigma i^{/2} \quad \textbf{(2.15)}$$

hold at iteration k, then update the matrix Bk by means of the BFGS formula (1.22) with Sk and yk given by (1.20). Otherwise, set Bk+i = Bk.

Here *Ok* is replaced by any quantity which is of the same order as the error e*, and, as in our previous paper, we use the optimality condition (IIZjjTitell + ||cfc||). Moreover, define

$$\cos\theta_k = \frac{s_k^T B_k s_k}{\|s_k\|\,\|B_k s_k\|}. \quad \textbf{(2.16)}$$

Prom Byrd and Nocedal (1989), the behavior of cos0* for BFGS updates can be described by the following theorem.

Theorem 2.1 *Let* $\{B_k\}$ *be generated by the BFGS formula (1.22) where, for all k>\, Sk ^0 and*

$$\frac{\%^T_o\wedge}{s_k\,s_k} \ge m > 0 \quad (2.17)$$

$$\frac{\|y_k\|^2}{y_k^T s_k} \le M. \quad (2.18)$$

Then, there exist constants /3\, 02,03 > **0** *such that, for any k* $\geq$ **1**, *the relations*

$$\cos Oj \quad \geq \quad fa \tag{2.19}$$

$$\beta_2 \leq \frac{\|B_j s_j\|}{\|s_j\|} \quad \leq \quad \beta_3 \tag{2.20}$$

hold for at least **f^fc]** *values of j* **€ [l,fc].**

This theorem refers to the iterates for which BFGS updating takes place, but since for the other iterates *Bk*+\ = £*, the theorem characterizes the whole sequence of matrices {£fc}. Theorem 2.1 states that, if s^y* is always sufficiently positive, in the sense that conditions (2.17) and (2.18) are satisfied, then at least half of the iterates at which updating takes place are such that *cosOj* is bounded away from zero and *BjSj* = O(||SJ||). Since it will be useful to refer easily to these iterates, we make the following definition.

Definition 2,1 *We define J to be the set of iterates for which BFGS updating takes place and for which (2.19) and (2.20) hold. We call J the set of "good iterates'*[7]*, and define* J_k = **Jfl {1,2,...,A;}.**

Note that if the matrices *Bk* are updated only a finite number of times, their condition number is bounded, and (2.19)-(2.20) are satisfied for all fc. Thus in this case all iterates are good iterates.

For the case when BFGS updating takes place an infinite number of times, we assume that all functions under consideration are smooth and bounded. If at a solution point x* the reduced Hessian $ZjW{+}Z_m$ is positive definite, then for all x_k in a neighborhood of *x the smallest eigenvalue of *Z^W^Zk* is bounded away from zero *(W^* is defined in (2.12)). We now show that in such a neighborhood with a* sufficiently small that Update Criterion I implies (2.17)-(2.18). For the case when $\overline{w}$^ is computed by Broyden's method. Using (2.13), (2.14) and (2.10), and since 7* converges to zero, we have**

$$\begin{aligned} s_k^T y_k &\geq C\|s_k\|^2 - O(\gamma_k^2\|s_k\|^2) - O(\gamma_k\|s_k\|^2) \\ &\geq m\|s_k\|^2, \end{aligned} \tag{2.21}$$

for some positive constants *C,m.* Also, from (2.11), (2.14) and (2.10) we have that

$$\begin{aligned} \|y_k\| &\leq O(\|s_k\|) + O(\gamma_k^2\|s_k\|) + O(\gamma_k\|s_k\|) \\ &\leq O(\|s_k\|). \end{aligned} \tag{2.22}$$

We thus see from (2.21)-(2.22) that there is a constant *M* such that for all *k* for which updating takes place

$$\frac{\|y_k\|^2}{y_k^T s_k} \leq M,$$

which together- with (2.21) shows that (2.17)-(2.18) hold when Broyden's method is used.

For $\overline{w}_k$ computed by the finite difference formula (2.2), from (1.20) and the Mean Value theorem there is a matrix $\hat{W}_k$ such that

$$\begin{aligned} y_k &= Z_{k+1}^T g_{k+1} - Z_k^T g_k - \overline{w}_k \\ &= Z_{k+1}^T \nabla L(x_{k+1}, \lambda_*) - Z_k^T \nabla \\ & \quad L(x_k, A_t) - a_k[Z_{\{} x_k + Y_{kPY})^T VL\{x_k + Y_k p_Y, A.) - 2\% VL(x_k, A.)] \\ &= (Z_{fc+}i - Z_k)^T VL(x_{k+1}, A.) + Zl(VL(x_{fc+}i, A,) - VL(s^*, A,)) \\ & \quad -\alpha_k[(Z_{(} x_k + Y_k p_Y) - Z_k)^T VL(x_k + Y_k p_Y, A.) \\ & \quad + Z_k^T(\nabla L(x_k + Y_k p_Y) A.) - VX(x_{fc}, A.))] \\ &= Zl\tilde{W}_k Z_k s_k + a_k Zl(\tilde{W}_k - \hat{W}_k) Y_{kPy} + O(a_k) \| s_k \| \\ &= Z_k^T \tilde{W}_k Z_k s_k + O\{a_k) \| s_k \|. \end{aligned}$$

assuming $Y_k py = 0\{a_k)$. Reasoning as before we see that (2.21) and (2.22) also hold in this case, and that (2.17)-(2.18) are satisfied in the case when finite differences are used. These arguments show that, in a neighborhood of the solution and whenever BFGS updating of B_k takes place, $s \backslash y_k$ is sufficiently positive, as stipulated by (2.17)-(2.18).

2.4. A Multiplier-free Approach for Choosing n_k.

We will choose $\backslash i$ so that for some $p > 0$,

$$\mathbf{MH^*)||\geq|A(^*)M^*)|+p||c(^*)||} \tag{2.23}$$

and show that this approach ensures a descent direction for the merit function. Moreover, for the good iterates J, it is a direction of strong descent.

Since d^ satisfies the linearized constraint (1.11) it is easy to show (see eq. (2.24) of Byrd and Nocedal (1991)) that the directional derivative of the $l\backslash$ merit function in the direction d* is given by

$$D\wedge_k(x_k; d_k) = gld_k - \text{WfclMlx}. \tag{2.24}$$

Also, the fact that the same right inverse of $A(x)^T$ is used in (1.12) and (1.24) implies that

$$g(x)^T Y(x) p_Y = \backslash(x)^T c(x). \tag{2.25}$$

We now show the following relation between Kuhn-Tucker points and merit functions with /i chosen by (2.23).

Theorem 2,1 *Assume that A(x) is of full column rank for all x € D and that Z(x) is norm bounded. If (p^x) is defined by (1.7) and fx satisfies (2.23) for all x* G *D, then D<t>^{x\d)* > 0 *for all d satisfying* $\bar{c}(x) + A(x)^T d = 0$ *if and only if* $\bar{x}$ *is a Kuhn-Tucker point.*

Proof. The proof is similar to the one in Fletcher (1987) for <£M(x) with /i > $\|\lambda(\bar{x})\|_\infty$. The *if part* follows from:

$$
\begin{aligned}
0 \le D\phi_\mu(\bar{x};d) &= \bar{g}(xfd\text{-}n\backslash\backslash c(\bar{x})\backslash\backslash i \\
&= g\{x)^T Z(\bar{x})p_z\text{-}_f x\backslash\backslash c(x)\backslash\backslash_1 + X\{\bar{x})^T c(\bar{x}) \\
&\le \bar{g}(x)^T \bar{Z}(x)p_z\text{-}p\backslash\backslash c(\bar{x})\backslash\backslash i \\
&\le g(\bar{x})^T Z(x)p_z \qquad (2.26)
\end{aligned}
$$

for all p_z € $H^n\sim^m$. This implies $Z(\bar{x})^T g\{x)^- = 0$. Now if, in addition, $c(\bar{x}) = 0$ then $\bar{x}$ is a Kuhn-Tucker point. If we assume $c(\bar{x})$ ^ 0 then we can show the contradiction:

$$
\begin{aligned}
0 \le Z\%(\bar{x};d) &= \backslash\{x)^T c(\bar{x}) - /i\|c(2)\|i \\
&\le -p\|c(S)\|i- \\
&< 0. \qquad (2.27)
\end{aligned}
$$

The *only if* part follows from substitution of the Kuhn-Tucker conditions:

$$
\begin{aligned}
Z(\bar{x})^T g(\bar{x}) &= 0 \\
c(\bar{x}) &= 0 \qquad (2.28)
\end{aligned}
$$

into the directional derivative:

$$
\begin{aligned}
D\hat{}(x;\bar{<}f) &= \bar{g}(x)^T Z(x)_{P_z}\text{-}fjL\backslash\backslash\bar{c}(x)\backslash\backslash iHx)^T c(\bar{x}) \\
&= 0. \qquad (2.29)
\end{aligned}
$$

D

To show strong descent directions for good iterates, we recall the decomposition (1.23) and use (2.25) to obtain

$$
\begin{aligned}
D\phi_{\mu_k}(x_k;d_k) &= g_k^T Z_k p_z - \mu_k\|c_k\|_1 + \lambda_k^T c_k \\
&= (Z_k^T g_k + \zeta_k w_k)^T p_z - \zeta_k w_k^T p_z - \mu_k\|c_k\|_1 + \lambda_k^T c_k. \qquad (2.30)
\end{aligned}
$$

Now from (1.23) we have that

$$BkSk = —OL_k(Z_k^T g_k + \text{Cifc\^{}A:)-} \qquad (2.31)$$

As shown in our previous paper,

$$\cos\theta_k = \frac{-(ZZgk + \{kWk)^T Pz}{\backslash\backslash 2\%gk + tkWk\backslash\backslash\backslash\backslash Pz\backslash\backslash'} \qquad (2.32)$$

If we satisfy the following property for fi_k:

$$H_k\backslash\backslash c_k\backslash\backslash \ge \underline{\backslash} Xlc_k\backslash + 2p\backslash\backslash c_k\backslash\backslash \qquad (2.33)$$

or, equivalently, from (2.25):

Wfellc*ll $\geq$ *igjYkPvl + 2p\\ck* **(2.34)**

then substituting in (2.30), leads to:

$$D\phi_{\mu_k}(x_k; d_k) \leq -\|Z_k^T g_k + \zeta_k w_k\| \, \|p_z\| \cos\theta_k - \zeta_k w_k^T p_z - 2\rho\|c_k\|_1. \tag{2.35}$$

Note also from (2.31) that

$$\frac{11^{**}11}{\|B_k s_k\|} = \frac{\text{lift } 11}{\|Z_k^T g_k + \zeta_k w_k\|}. \qquad (2.3\text{gX})$$

We now concentrate on the good iterates J, as given in Definition 2.1. If *j* G J, we have from (2.36) and (2.20) that

$$\frac{1}{\beta_3}\|Z_j^T g_j + \zeta_j w_j\| \leq \|p_z^{(j)}\|, \text{ - } \underset{\mu_2}{\overset{1}{ir}}\backslash\backslash^{z}i_{\text{.}}\ 9j\ +\ CjWjll \tag{2.37}$$

Using this and (2.19) in (2.35) we obtain, for *j* 6 *J*,

$$\begin{aligned} D\phi_{\mu_j}\, ix_j d\ _j) \ &\leq\ -\frac{1}{\beta_3}\ \backslash\backslash Zg_j\ +_j w_j\|^2\cos\theta_j - \zeta_k w_j^T p_z^{(j)} - 2\rho\|c_j\|_1 \\ &\leq\ \text{-}\wedge\backslash\backslash zj_{9j}f\ \text{-}\ \ {}^2Si\wedge i_{\{g}T_{ZjWj)}\ \ -\ CjWj_{pz}\mu)\ -\ mej\ \|_1, \end{aligned}$$

where we have dropped the non-positive term — *tf cosQJ\\WJ*^{2}*/fa.* Since we can assume that /% > 1 (it is defined as an upper bound in (2.20)), we have

$$D\phi_{\mu_j}(x_j; d_j) \leq -\frac{}{\beta}\ \|Z_j^T g_j\|^2 + \ \ \zeta_j \cos\theta_j |g_j^T Z_j w_j| - 2\rho\|c_j\|_1 \ldots p_z^{(j)}$$

It is now clear that if

2Cj cos *6j\gjZjWj*| - *CjwjpV** $\leq$ *p\\cj* ||i, **(2.38)**

then for all *j* G J,

DϕH(xy,dj) $\leq$ - ^ l l ^ l l ^{2} - ***pWcjh.*** **(2.39)**

This means that if (2.38) holds, then for the good iterates, *j* € J, the search direction *dj* is a strong direction of descent for the *t* merit function in the sense that the first order reduction is proportional to the KKT error.

We will choose £* so that (2.38) holds for *all* iterations. To see how to do this we note from (1.23) that

$$p_z = -B_k^{-1} Z_k^T g_k - \zeta_k B_k^{-1} w_k,$$

so that for $j = k$ (2.38) can be written as

$$Ck[2cos6_k\backslash glZ_kw_k\backslash + w^T{}_kBl^xZlg_k + CkwlB\wedge^lw_k] \leq p||c_{fc}||i. \qquad \textbf{(2.40)}$$

It is clear that this condition is satisfied for a sufficiently small and positive value of £*. Specifically, at the beginning of the algorithm we choose a constant $p > 0$ and, at every iteration fc, define

$$Ct = \min\{l, C\hat{fc}\} \qquad (2.41)$$

where $\hat{0}t$ is the largest value that satisfies (2.40) as an equality.

The penalty parameter /z* must satisfy (2.23), so we define it at every iteration of the algorithm by

$$\mu_k = \begin{cases} \mu_{k-1} & \text{if } \mu_{k-1}\|c_k\|_1 \geq |g_k^T Y_k p_Y| + 2\rho\|c_k\|_1 \\ |g_k^T Y_k p_Y|/\|c_k\|_1 + 3\rho & \text{otherwise.} \end{cases} \qquad \textbf{(2.42)}$$

Note that for $c_k = 0$, jjL_k = /Zfc_i and thus fx_k is only updated when $c_k \wedge 0$.

The damping factor £* and the updating formula for the penalty parameter fi_k have been defined so as to give strong descent for the good iterates J. We now show that they ensure that the search direction is also a direction of descent (but not necessarily of strong descent) for the other iterates, k & J. Since (2.38) holds for all iterations by our choice of Cfc> we have in particular

$$-\zeta_k w_k^T p_Z \leq \rho\|c_k\|_1.$$

Using this and (2.42) in (2.35), we have

$$D\phi_{\mu_k}(x_k; d_k) \leq -\|Z_k^T g_k + \zeta_k w_k\|\,\|p_Z\| \cos\theta_k - \rho_k\|c_k\|_1. \qquad \textbf{(2.43)}$$

The directional derivative is thus non-positive. Furthermore, since $w_k = 0$ whenever $c_k = 0$ (regardless of whether w_k is obtained by finite differences or through Broyden's method), it is easy to show that this directional derivative can only be zero at a stationary point of problem (1.1)-(1.2).

2.5. The Algorithm

Using the modifications of the reduced Hessian algorithm for the multiplier-free method, we now give a complete description of the algorithm. As with the previous paper, the algorithm includes an approximation for the cross term using Broyden's method and finite differences, and based on the relative sizes of p_Y and p_Z. Calculation of the cross term and updating of the reduced Hessian proceed in the same manner as in our previous paper.

Algorithm I

1. **Choose constants 77 E (0,1/2), $p > 0$ and r, r^f with $0 < r < r' < 1$, and positive constants F and j_{id} for conditions (2.9) and (2.15), respectively. For conditions (2.10) and (2.14), select a summable sequence of positive numbers {7*}. Set $k := 1$ and choose a starting point xi, an initial value .(JL\ > 0 for the penalty parameter, an (n — m) x (n — m) symmetric and positive definite starting matrix B\ and an (n — m) x n starting matrix S\.**

2. **Evaluate /*,</*, c* and Ak, and compute % and Z*.**

3. **Set *findiff* = *false* and compute p_Y by solving the system**

$$(AlY_k)p_Y \quad = \quad -c*. \qquad \text{(range space step)} \tag{2.44}$$

4. **Calculate tu* using Broyden's method, from equations (2.8) and (2.9).**

5. **Choose the damping parameter C,k from equations (2.40) and (2.41) and compute p_z from**

$$B_k p_z = -\backslash^z k9k + CkWk]- \qquad \text{(null space step)} \tag{2.45}$$

6. **If (2.15) is satisfied and (2.14) is *not* satisfied, set *findiff* = *true* and recompute *Wk* from equation (2.1).**

7. **If *findiff* = *true* use this new value of w^ to choose the damping parameter £* from equations (2.40) and (2.41) and recompute p_z from equation (2.45).**

8. **Define the search direction by**

$$d_k \;=\; Y_k p_Y \;+\; Zfcp_z, \tag{2.46}$$

and set a& = 1.

9. **Test the line search condition**

$$<t>n_k(xk + <*kdk) \leq <l>n_k\{xk) + vakDcfr\wedge ixkidk). \tag{2.47}$$

10. **If (2.47) is not satisfied, choose a new a* E [rak,r'ak] and go to 9; otherwise set**

$$Xfc+i\wedge fc \;+\; afcd*. \tag{2.48}$$

11. **Evaluate /*+i,0*4.1,c*+i, $A*_+$i, and compute Yjk4i and Z*+i.**

12. **Update /x* so as to satisfy (2.42).**

13. **Update £*+! using equations (2.5) to (2.7). If *findiff* = *false* calculate tJ* by Broyden's method through equations (2.8) and (2.10); otherwise calculate *Wk* by (2.2).**

14. If $s\%y_k \leq 0$ or if (2.15) is not satisfied, set -B^+i = B_k. Else, compute

$$s^* = <**Pz, \tag{2.49}$$

$$Vk = Zl+_{ig}\{x_k+i) - Zlg\{x_k) - \overline{w}_k, \tag{2.50}$$

and compute B_k+_X by the BFGS formula (1.22).

15. Set A; := k + 1, and go to 3.

3. Convergence Results

In this section we summarize several convergence results for Algorithm I. Many of the results of the our previous paper carry over directly and are thus stated without proof. Nevertheless, there are some important departures which are noted as well.

3.1. Semi-Local Behavior of the Algorithm.

We first show that the merit function <*f*>^ decreases significantly at the good iterates J, and that this gives the algorithm a weak convergence property. To establish the results of this section we restate the following assumptions from our previous paper.

Assumptions 3.1 The sequence $\{x_k\}$ generated by Algorithm I is contained in a convex set *D* with the following properties.

(I) The functions / : R^n -> R and c : R^n -* R^m and their first and second derivatives are uniformly bounded in norm over *D*.

(II) The matrix *A(x)* has full column rank for all *x* € *D*, and there exist constants 70 and *fa* such that

$$WYixnAixfYix)\}-^{1}\wedge\wedge, \qquad ||Z(s)||<\underline{i}flb, \tag{3.1}$$

for all *x* € *D*.

(III) For all $k \geq 1$ for which B_k is updated, (2.17) and (2.18) hold.

(IV) The correction term to* is chosen so that there is a constant K > 0 such that for all

$$\|w_k\| \leq KllcfeU^{1/2}. \tag{3.2}$$

The following result from our previous paper concerns the good iterates J, as given in Definition 2.1.

Lemma 3.1 *If Assumptions 3.1 hold and if fij = fj, is constant for all sufficiently large j, then there is a positive constant* 7^ *such that for all large j* G J,

$$\phi_\mu(x_j) - \phi_\mu(x_{j+1}) \geq 7M\,[11\hat{\ }j11^2 + IMh] \bullet \tag{3.3}$$

It is now easy to show that the penalty parameter settles down, and that the set of iterates is not bounded away from stationary points of the problem.

Theorem 3.2 *If Assumptions 3.1 hold, then the weights* {/x/k} *are constant for all sufficiently large k and]imM$_k$->oo(\\Zk 9k* + l|c*ll) = 0.

Proof. First note that by Assumptions 3.1 (I)-(II) and (2.25) that {Ifffl*p$_Y$|/||c*||i} = {|^jf^{c}fcl/ll^c*lli} ^ {11^*11} is bounded. Therefore, since the procedure (2.42) increases /U* by at least *p* whenever it changes the penalty parameter, it follows that there is an index fco and a value /i such that for all *k* > fco, Wb = A^{4suc}h *kat Ml|c/k||i ≥ |A£cfc| + 2p||c*|ji. If BFGS updating is performed an infinite number of times, by Assumptions 3.1-(III) and Theorem 2.1 there is an infinite set *J* of good iterates, and by Lemma 3.1 and the fact that *<f>n(xk)* decreases at each iterate, we have that for *k* > &o,

$$\begin{aligned}\phi_\mu(x_{k_0}) - \phi_\mu(x_{k+1}) &= \sum_{j=k_0}^{k} (\phi_\mu(x_j) - \phi_\mu(x_{j+1})) \\ &\geq \sum_{j6Jn[k_o,k]} (\phi_\mu(x_j) - \phi_\mu(x_{j+1})) \\ &\geq \gamma_\mu \sum_{jeJn[k_o,k]} [\|Z_j^T g_j\|^2 + \|c_j\|_1].\end{aligned}$$

By Assumption 3.1-(I) ^$_M$(x) is bounded below for all **x E D,** so the last sum is finite, and thus the term inside the square brackets converges to zero. Therefore

$$\lim_{j\in J} (P| j \hat{\ } +1\hat{\ }110=0. \tag{3.4}$$

If BFGS updating is performed a finite number of times then, as discussed after Definition 2.1, all iterates are good iterates, and in this case we obtain the stronger result

.lim (H^ffjtH + Hcfclli) = 0.

□

3.2. Local Convergence

In this section we show that if *x+* is a local minimizer that satisfies the second order optimality conditions, and if the penalty parameter /x* is chosen large enough, then x* is a point of attraction for the sequence of iterates *{xk}* generated by Algorithm I. To prove this result we will make the following assumptions. In what follows *G* denotes the reduced Hessian of the Lagrangian function, i.e.

$$G_k = Z_k^T \nabla_{xx}^2 L(x_k, \lambda_k) Z_k. \tag{3.5}$$

Assumptions 3.2 The point z* is a local minimizer for problem (1.1)-(1.2) at which the following conditions hold.

(1) The functions / : R^n -> R and *c* : R^n -» R^m axe twice continuously differentiable in a neighborhood of x*, and their Hessians are Lipschitz continuous in a neighborhood **of x_*.**

(2) The matrix *A(x+)* has full column rank. This implies that there exists a vector A* G R^m such that

VL(z*, A,) = *g(x_m)* + *A{x*)** = 0.

(3) For all *q e* R^n~^{m}, *q* ^ 0, we have $q^T G^* q$ > 0.

(4) There exist constants 70, /?o and 7_C such that, for all *x* in a neighborhood of x*,

WYixHAixfYix^WK-to, ***\\Z(x)\\≤f3o,*** **(3.6)**

and

\\[Y(x)Z(x)]-^{1}\\≤y_c. (3.7)

(5) *Z(x)* and *X(x)* are Lipschitz continuous in a neighborhood of x«, i.e. there exist constants j_z and 7^ such that

$$\|\lambda(x) - \lambda(z)\| \le \gamma_\lambda \|x - * \text{ I I },\tag{3.8}$$

\\Z(x) - Z(z) ≤ $_7$z||x-z||, (3.9)

for all *x, z* near x».

Note that (1), (3) and (5) imply that for all *(x, X)* sufficiently near (x,,A»), and for all *q*€$R^{n"m}$,

m\\q\\$^2$≤$q^T$G(x,\)q<M\\q\\$^2$, (3.10)

for some positive constants m, M. We also note that Assumptions 3.2 ensure that the conditions (2.17)-(2.18) required by Theorem 2.1 hold whenever BFGS updating takes place in a neighborhood of x*. Therefore Theorem 2.1 can be applied in the convergence analysis.

The following lemma is proved by Xie (1991) for very general choices of *Y* and Z. Their result generalizes Lemma 4.1 of Byrd and Nocedal (1991); see also Powell (1978).

Lemma 3.3 *// Assumptions 3.2 hold, then for all x sufficiently near x**

$$\text{Till* - x.}\| \leq \|c(x)\| + \|Z\{x)^T g\{x)\| \leq {}_{l2}\|x - x.\|, \qquad (3.11)$$

for some positive constants 71,72 •

This result states that, near z*, the quantities $c(x)$ and $Z(x)^T g(x)$ may be regarded as a measure of the error at x. The next lemma states that, for a large enough weight, the merit function may also be regarded as a measure of the error.

Lemma 3.4 *Suppose that Assumptions 3.2 hold at* x«. *Then for any \x satisfying (2.23) there exist constants* 73 > 0 *and* 74 > 0, *such that for all x sufficiently near x**

$$\text{TSII* " *.}\|^2 \leq M^x) \sim M^{x}") \leq 74\ [\|Z(xf_9(x)\|^2 + \|c(x)\|ij\ . \qquad (3.12)$$

Proof. To show the left inequality holds we can write:

$$
\begin{aligned}
*_{„}(*)-*_{„}(*.) &= /(*)+/i\|c(z)\|_1-/(*,) && (3.13)\\
&= /(*) + X(xfc(x) + |AI\|C(X)\|I - X(xfc(x)\} - /(x.) && (3.14)\\
&\geq L(x, A.) + (A(x) - \backslash(x,)fc(x) + p\|c(x)\|i - /(x.) && (3.15)\\
&\geq L(x,A.) + |\|c(x)\|i-/(x.) && (3.16)\\
& && (3.17)
\end{aligned}
$$

where the last inequality follows for all x sufficiently near x^*. Expanding the last inequality in a Taylor series leads to:

$$
\begin{aligned}
\phi_\mu(x) - \phi_\mu(x_*) \geq\ & \nabla L(x_*, \lambda_*)^T(x - x_*) + \frac{1}{2}(x - x_*)^T \nabla^2_{xx} L(x_*, \lambda_*)(x - x_*)\\
& + f\ \|c(x)\|_1 + \wedge\|c(x)\|^2 - \wedge\|c(x)\|^2 + O(\|x - x.\|)^3 \qquad (3.18)
\end{aligned}
$$

Now we note that

$$\wedge Mx)f = {}^U\text{-}\frac{}{2}\{x - x.)^T A.jg(x - x.) + O(\|x - x.\|)^3. \qquad (3.19)$$

In Lemma 4.2 of Byrd and Nocedal (1991) it is shown that if Assumptions 3.2 are satisfied there exist sufficiently large values of v such that:

$$\bullet\ |(x - x.)^T(V^2_{xx}L(x_b, A.) + vA.A^*_*)(x - x.) \geq 2_{73}\|a; - x.f \qquad (3.20)$$

Now since there exists a $K_c > 0$ such that $\|c(a;)\|i \leq K_c\|x - x_m\|$ we have for $\|i - x,\| \leq p/(2vK_c)$:

$$
\begin{aligned}
\phi_\mu(x) - \phi_\mu(x_*) &\geq 2\gamma_3\|x - x_*\|^2 + \wedge\ \|c(x)\|_1 + O(\|x\ )^3 && (3.21)\\
&\geq 73\text{lk-ar.ll}^2 && (3.22)\\
& && (3.23)
\end{aligned}
$$

for all x sufficiently close to x*. The right inequality follows directly from:

$$Ms)-</>*(*\bullet) = /(*) + H|c(x)||i-/(x*) \quad (3.24)$$
$$= L(x, A) - f(x.) + Mk(*)lli \text{ "} Hxfc(x)\} \quad (3.25)$$
$$\leq O(\|x - x4^2) + p\backslash\backslash c(x)h \quad (3.26)$$
$$\leq \gamma_4[\|Z(x)^T{}_9(a:)\|^2 + \|c(x)\|_1] \quad * \quad (3.27)$$

D

Note that the left inequality in (3.12) implies that for a sufficiently large value of the penalty parameter, the merit function will have a strong local minimizer at x*. We will now use the descent property of Algorithm I to show convergence of the algorithm. However, due to the non-convexity of the problem, the line search could generate a step that decreases the merit function but that takes us away from the neighborhood of x*. To rule this out we make the following assumption.

Assumption 3.3 The line search has the property that, for all large A;, <^((1 — *9)xk + Oxk+i)* $\leq$ 0/x(#fc) f°r all *6* E [0,1]. In other words, x/t+i is in the connected component of the level set *{x* : </>$_M$(x) $\leq$ *4>p{xk)}* that contains x*.

There is no practical line search algorithm that can guarantee this condition, but it is likely to hold close to x*. Assumption 3.3 is made by Byrd, Nocedal and Yuan (1987) when analyzing the convergence of variable metric methods for unconstrained problems, as well as by Byrd and Nocedal (1991) in the analysis of Coleman-Conn (1984) updates for equality constrained optimization.

Lemma 3.5 *Suppose that the iterates generated by Algorithm I are contained in a convex region D satisfying Assumptions 3.1. If an iterate Xk_Q is sufficiently close to a solution point* x* *that satisfies Assumptions 3.2, and if the weight* /i^$_0$ *is large enough, then the sequence of iterates converges to x*.*

Proof. The proof is virtually identical to the one given in our previous paper. By Assumptions 3.1 (I)-(II) and (1.24) we know that {||Afc||} is bounded. Therefore the procedure (2.42) ensures that the weights /x* are constant, say /ijb = /i for all large fc. Moreover, if an iterate gets sufficiently close to x*, we know by (2.42) and by the continuity of A that (2.23) is satisfied. For such a value of /i, Lemma 3.2 implies that the merit function has a strict local minimizer at x*. Now suppose that once the penalty parameter has settled, and for a given *e* > 0, there is an iterate Xk_0 such that

$$\|x_{k_0} - x_*\| \leq \frac{\gamma_3}{\gamma_2\gamma_4\hat{\gamma}_0}\epsilon^2,$$

where 70 is such that || • ||i $\leq$ 70II • II- Assumption 3.3 shows that for any $k \geq k_0$, x* is in the connected component of the level set of x*$_0$ that contains Xfc$_0$, and we can assume that c is small enough that Lemmas 3.3 and 3.4 hold in this level set. Thus since

$4>iii^xk)\leq <j>n(^xk_o)$ for $\Delta; > /to$, and since we can assume that $\|£j\hat{}<feoll \leq 1>$ we have from Lemmas 3.3 and 3.4, for any $k \geq ko$

$$\begin{aligned}
\|x_k - x_*\| &\leq \gamma_3^{-\frac{1}{2}}(\phi_\mu(x_k) - \phi_\mu(x_*))^{\frac{1}{2}} \\
&\leq \gamma_3^{-\frac{1}{2}}(\phi_\mu(x_{k_0}) - \phi_\mu(x_*))^{\frac{1}{2}} \\
&\leq \left(\frac{\gamma_4}{\gamma_3}\right)^{\frac{1}{2}} \left[\|Z_{k_0}^T g_{k_0}\|^2 + \|c_{k_0}\|_1\right]^{\frac{1}{2}} \\
&\leq (\hat{}\ )^{\frac{1}{2}} \left[\|Z_{k_0}^T g_{k_0}\|^2 + \hat{\gamma}_0\|c_{k_0}\|\right]^{\frac{1}{2}} \\
&\leq \left(\frac{\gamma_2\gamma_4\hat{\gamma}_0}{\gamma_3}\|x_{k_0} - x_*\|\right)^{\frac{1}{2}} \\
&\leq \epsilon.
\end{aligned}$$

This implies that the whole sequence of iterates remains in a neighborhood of radius e of $x+$. If e is small enough we conclude by (3.12), by the monotonicity of $\{(f>n\{x_k)\}$ and Theorem 4.2 that the iterates converge to x».

D

3.3. R-Linear Convergence.

For the rest of the paper we assume that the iterates generated by Algorithm I converge to x«, which implies that for all large k and some $p > 0$, /x* = /x and

$$»\|c(x)\|\geq\|(xfc(x)\|+pMx)\| \tag{3.28}$$

The analysis that follows depends on how often BFGS updating is applied, and to make this concept precise we define U to be the set of iterates at which BFGS updating takes place,

$$U = \{k : B_M = BFGS(B_k, s_k, y_k)\}, \tag{3.29}$$

and let

$$U_k = UD\ \{1,2, ..,\&\}. \tag{3.30}$$

The number of elements in U_k will be denoted by $\backslash U_k\backslash$. The following result from our previous paper carries over directly to the multiplier-free method.

Theorem 3.6 *Suppose that the iterates $\{x_k\}$ generated by Algorithm I converge to a point x^* that satisfies Assumptions 3.2. Then for any k £U and any $j \geq k$*

$$\|x_j - x_*\| \leq Cr^{|U_k|}, \tag{3.31}$$

for some constants $C > 0$ and $0 \leq r < 1$.

This result implies that if *{\Uk\/k}* is bounded away from zero, then Algorithm I is R-lineaxly convergent. However, BFGS updating could take place only a finite number of times, in which case this ratio would converge to zero. It is also possible for BFGS updating to take place an infinite number of times, but every time less often, in such a way that *\U_k\/k* —¥ 0. We therefore need to examine the iteration more closely.

We make use of the matrix function *ip* defined by

$$\psi(B) = tr\{B) - \ln(\text{cfct}(B)), \tag{3.32}$$

where *tr* denotes the trace, and *det* the determinant. It can be shown that

lncond(B)<V>(£), (3.33)

for any positive definite matrix *B* (Byrd and Nocedal (1989)). We also make use of the weighted quantities

$$\tilde{V}k = G7^{l/2}y_k, \qquad \tilde{s}_k = G^lJ^2s_k, \tag{3.34}$$

$$\tilde{B}_k = G;^{1/2}B_{fc}G;^{1/2}, \tag{3.35}$$

$$\cos\tilde{\theta}_k = \frac{\tilde{s}_k^T\tilde{B}_k\tilde{s}_k}{\|£*«*\|\|\|**\|}, \tag{3.36}$$

and

$$\tilde{q}_k = 2g\wedge_{\tilde{s}_k s_k} \tag{3.37}$$

One can show (see eq. (3.22) of Byrd and Nocedal (1989)) that if B_k is updated by the BFGS formula then

$$\begin{aligned}\psi(\tilde{B}_{k+1}) &= \psi(\tilde{B}_k) + \frac{\|\tilde{y}_k\|^2}{\tilde{y}_k^T\tilde{s}_k} - 1 - \ln\frac{\tilde{y}_k^T\tilde{s}_k}{\tilde{s}_k^T\tilde{s}_k} + \ln\cos^2\tilde{\theta}_k \\ &\quad + \left[1 - \frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k} + \ln\frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k}\right].\end{aligned} \tag{3.38}$$

This expression characterizes the behavior of the BFGS matrices B_{ky} and will be crucial to the analysis of this section. However before we can make use of this relation we need to consider the accuracy of the correction terms. We begin by showing that when finite differences axe used to estimate w_k and TU\, these axe accurate to second order.

Lemma 3.7 *// at the iterate x_k, the corrections w_k and $\overline{w_k}$ are computed by the finite difference formulae (2.1)-(2.2), and if x_k is sufficiently close to a solution point* z* *that satisfies Assumptions 3.2, then*

«»* = O(lbvll), (3-39)

IK - Z,[r]W.y_fe p_Y|| = *O{a_k\\p_Y\\)* (3.40)

and

$$\|\overline{w}_k - \alpha_k Z^T W_* Y_k p_Y\| = O(\sigma_k\|p_Y\|). \tag{3.41}$$

Proof. The proof requires only a minor modification of the same property proved in the previous paper. Recalling that VL(z, A) = $g(x)$ + A(x)A, we have from (2.1) that

$$
\begin{aligned}
w_k &= Z(x_k + Y_k\bar{p}_Y)^T g\{x_k + Y_k p_Y) - Z(x_k)^T g(x_k) \\
&= Z(x_k + Y_k p_Y)^T VL(x_k + Y_k p_Y, \text{A,}) - Z(x_k)^T VL(x_k, \text{A,}) \\
&= (Z(x_k + Y_k p_Y) - Z(x_k))^T VL(x_k + Y_k p_Y, \backslash *) \\
&\quad + Z_k^T \left[\int_0^1 V^2_{xx} L\{x_k + rY_k p_Y, \text{A,)rfr} \right] Y_k p_Y \\
&\equiv Z_k^T \overline{W}_k Y_k p_Y + (Z(x_k + \text{npy}) - \text{Z(x*)})^{\text{r}} \text{VL(a*} + Y_k p_Y, \text{A,}) \\
&= Z_k^T \overline{W}_k Y_k p_Y + O(\sigma_k) \|p_Y\| \qquad (3.42)
\end{aligned}
$$

The above result follows for x_k in the neighborhood of £* where (3.6)-(3.9) hold because:

$$VL(x_k + Y_k p_Y, \text{A.}) = \text{O}(\|\text{x} - x_m\backslash\backslash) + \text{O}(|\text{b}_\text{Y}\|) = \text{O}(\text{a}_{\text{fc}}) \qquad (3.43)$$

where a_k is defined by (1.29). Also a simple computation shows that

$$[ZlW_k - Z?W.]Y_{kPY} = \textbf{OVibllPvll).)} \qquad \textbf{(3.44)}$$

Using these facts in (3.42) yields the desired result (3.40). To prove (3.41), we only note that $a_k \leq 1$, and reason in the same manner. D

Next we show that the condition number of the matrices B_k is bounded, and that at the iterates U at which BFGS updating takes place the matrices B_k are accurate approximations of the reduced Hessian of the Lagrangian.

Theorem 3.8 *Suppose that the iterates $\{x_k\}$ generated by Algorithm I converge to a solution point x* that satisfies Assumptions 3.2. Then* {‖B^‖} *and* $\{\backslash\backslash B^{\wedge^l}\backslash\backslash\}$ *are bounded, and for allkeU*

$$\|(B_k - Z^\wedge \quad Z_*)p_Z\| = o(\|d_k\|). \qquad (3.45)$$

Proof. Again, the proof follows along the same lines as the one in our previous paper, but with slight modification. Consider only iterates k for which BFGS updating of Bk takes place. We have from (2.50), (2.48), (2.46), (2.12) and (2.49)

$$
\begin{aligned}
y_k &= Zj_{+1} g_{k+1} - Zlg_k - \overline{w}_k \\
&= Z_{k+1}^T \nabla L(x_{k+1}, X,) - Z][VL(x_k, X,) - \overline{w}_k \\
&= (Z_{k+1} - Z_k f VL(x_{k+1}, \text{A.}) + \text{ZftVLfo+i, A.}) - VL(x_k, \text{A.})) - \overline{w}_k \\
&= (Z_{k+1} - Z_k)^T VL\{x_{k+u}, \text{A,}) + [\text{z j jf}_0^1 V^2_{xx} L(x_k + Ta_k d_k, \text{A,)rfr}] \; a_k d_k - \overline{w}_k \\
&= ct_k Zl\tilde{W}_k\{Z_{kPz} + Y_k p_Y) - \overline{w_k} + \text{O}(<7_{\text{fc}})(\|\text{a}_{\text{fc}}\| + \text{a}_k \|p_Y\|) \\
&= Z\bar{l}W_k Z_k s_k + a_k\{Zl\tilde{W}_k - ZT\backslash V.)Y_k p_Y + (a_k ZjW.Y_k p_Y - \overline{w}_k) \\
&\quad + O(a_k)(\backslash\backslash s_k\backslash\backslash + a_k \backslash\backslash p_Y \backslash\backslash). \qquad (3.46)'
\end{aligned}
$$

Since $\overline{w}_k$ can be computed by Broyden's method or by finite differences, we consider these two cases separately.

Part I. We first assume that $\overline{w}_k$ is determined by Broyden's method. A simple computation shows that $\|Z_*^T[\tilde W_k - Z_k^T W_*]\| = O(\sigma_k)$, and from (2.10) we have that $\overline{w}_k = O(\|p_Y\|/\gamma_k)$. Using this and Assumptions 3.2 in (3.46) we have

$$\begin{aligned} y_k &= Z_k^T\tilde W_k Z_k s_k + (\sigma_k + 1 + 1/\gamma_k)O(\alpha_k\|p_Y\|) + O(\sigma_k)\|s_k\| \\ &= (Z_k^T\tilde W_k Z_k - G_*)s_k + G_* s_k + (\sigma_k + 1 + 1/\gamma_k)O(\alpha_k\|p_Y\|) + O(\sigma_k)\|s_k\|. \end{aligned} \tag{3.47}$$

Recalling (3.34) and noting that $\tilde y_k^T \tilde s_k = y_k^T s_k$ we have

$$\tilde y_k^T \tilde s_k = s_k^T(Z_k^T\tilde W_k Z_k - G_*)s_k + \|\tilde s_k\|^2 + (\sigma_k + 1 + 1/\gamma_k)O(\alpha_k\|p_Y\|)\|\tilde s_k\| + O(\sigma_k)\|s_k\|^2,$$

since $\|\tilde s_k\|$ and $\|s_k\|$ are of the same order. Therefore

$$\begin{aligned} \frac{\tilde y_k^T \tilde s_k}{\|\tilde s_k\|^2} &= 1 + \frac{s_k^T(Z_k^T\tilde W_k Z_k - G_*)s_k}{\|\tilde s_k\|^2} \\ &\quad + (\sigma_k + 1 + 1/\gamma_k)O\left(\frac{\|\alpha_k p_Y\|}{\|\tilde s_k\|}\right) + O(\sigma_k) \\ &= 1 + O(\sigma_k) + (\sigma_k + 1 + 1/\gamma_k)O\left(\frac{\|\alpha_k p_Y\|}{\|\tilde s_k\|}\right) \end{aligned} \tag{3.48}$$

Similarly from (3.47) and (3.34) we have

$$\begin{aligned} \tilde y_k^T \tilde y_k \le\ & \|(Z_k^T\tilde W_k Z_k - G_*)s_k\|^2\|G_*^{-1}\| \\ & + 2(1 + O(\sigma_k))\|(Z_k^T\tilde W_k Z_k - G_*)s_k\|\,\|G_*^{-1/2}\|\,\|\tilde s_k\| + (1 + O(\sigma_k))^2\|\tilde s_k\|^2 \\ & + 2(\sigma_k + 1 + 1/\gamma_k)O(\|\alpha_k p_Y\|)\|G_*^{-1/2}\|\left((1 + O(\sigma_k))\|\tilde s_k\| + \|(Z_k^T\tilde W_k Z_k - G_*)s_k\|\|G_*^{-1/2}\|\right) \\ & + (\sigma_k + 1 + 1/\gamma_k)^2 O(\|\alpha_k p_Y\|)^2, \end{aligned} \tag{3.49}$$

and thus

$$\begin{aligned} \frac{\|\tilde y_k\|^2}{\|\tilde s_k\|^2} \le\ & 1 + O(\sigma_k) + (\sigma_k + 1 + 1/\gamma_k)(1 + \sigma_k)O\left(\frac{\|\alpha_k p_Y\|}{\|\tilde s_k\|}\right) \\ & + (\sigma_k + 1 + 1/\gamma_k)^2 O\left(\frac{\|\alpha_k p_Y\|^2}{\|\tilde s_k\|^2}\right). \end{aligned} \tag{3.50}$$

At this point we invoke the update criterion, and note from (2.14) that if BFGS updating of B_k takes place at iteration k, then $\|\alpha_k p_Y\| \le \gamma_k^2\|s_k\|$ where $\{\gamma_k\}$ is summable. Using this, the assumption that σ_k converges to zero, and (3.48) we see that for large k

$$\frac{\tilde y_k^T \tilde s_k}{\|\tilde s_k\|^2} = 1 + O(\sigma_k + \gamma_k), \tag{3.51}$$

and using (3.50)

$$\frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} = 1 + O(\sigma_k + \gamma_k).$$

Therefore

$$\frac{\|\tilde{y}.\|^2}{y_k \tilde{s}_k} = \frac{\|\tilde{y}\wedge\|^2 1!5\wedge\|^2}{\|*\tilde{k}\|r \; \tilde{y}_k^T \tilde{s}_k} = 1 + \tilde{C}J(a* + 7*)- \qquad (3.52)$$

We now consider $x/>(\tilde{B}_k+i)$ given by (3.38). A simple expansion shows that for large fc, ln(l + $O(a_k$ + 7fc)) = O(CTA: + 7*). Using this, (3.51) and (3.52) we have

$$4>(\tilde{B}_M) = 1>(\tilde{B}_k) + O\{o_k + _{lk}) + \ln\cos^2 \S_k + [1 - \_\text{»} \text{—H} - \ln - \wedge - 1 . \quad \text{L} \quad \cos^2 0k \quad \cos^2 \theta J \qquad (3.53)$$

Note that for $x \geq 0$ the function $1 - x + \ln x$ is non-positive, implying that the term in square brackets is non-positive, and that $\ln\cos^2 \bar{0}_k$ is also non-positive. We can therefore delete these terms to obtain

$$iK\tilde{B}_M) \leq *l*\{\tilde{B}_k) + O(a_k + 7.). \qquad (3.54)$$

Before proceeding further we show that a similar expression holds when finite differences are used.

Part II. Let us now consider the iterates k for which updating takes place and for which $\overline{w}_k$ is computed by finite differences. In this case (2.15) holds. Again we begin by considering (3.46),

$$y_k = Z j l \wedge Z \wedge + a f c \wedge \wedge_k - Z_*^T W_*) Y_k p_Y + (\alpha_k Z_*^T W_* Y_k p_Y - \overline{w}_k) + O(\sigma_k)(\|s_k\| + \alpha_k \|p_Y\|).$$

Using (3.41) the second and third terms are of order a*(a*||pY||)- Thus

$$\begin{aligned} y_k &= Z_k^T \tilde{W}_k Z_k s_k + O(\sigma_k)(\|s_k\| + \alpha_k \|p_Y\|) \\ &= \{Zl\tilde{W}_k Z_k - G.)s_k + G.s_k + O(a_k)(\|s_k\| + a*\|p_Y\|). \end{aligned} \qquad (3.55)$$

Noting once more that $\tilde{y}\%\tilde{s}_k = y\wedge Sk$ and recalling the definition (3.34) we have

$$\tilde{y}lh = s\backslash\{Zl W_k \tilde{Z}_k - G.)8_k + \|h\|^2 + O(a_k)(\|\tilde{s}_k\|^2 + \alpha_k \|p_Y\| \|\tilde{s}_k\|),$$

since ||i^|| and ||s*|| are of the same order. Therefore

$$\begin{aligned} \frac{\tilde{y}js k}{P\wedge F} &- 1 + \frac{s^T{}_k\{Zl\tilde{W}_k Z_k - G.)s_k}{P \wedge P} + 0\{ak)\left(l + \frac{\|\alpha_k p_Y\|}{i \wedge r}\right) \\ &= 1 + O(\sigma_k) + O\left(\sigma_k \frac{\|\alpha_k p_Y\|}{\|\tilde{s}_k\|}\right). \end{aligned} \qquad (3.56)$$

Similarly from (3.55) and (3.34) we have

$$\tilde{y}_k^T\tilde{y}_k \le \|(Z_k^T W_k Z_k - G_*)s_k\|^2 \|G_*^{-1}\|$$
$$+2(1 + O(\alpha_k))\|(Z_k^T \tilde{W}_k Z_k - G_*)s_k\| \; \|G_*^{-1/2}\| \; \|\tilde{s}_k\| + (1 + O(\alpha_k))\|\tilde{s}_k\|^2$$
$$+\sigma_k O\left(\|\alpha_k p_Y\| \|G_*^{-\frac{1}{2}}\| \; [(1 + O(\alpha_k))\|\tilde{s}_k\| + \|(Z_k^T \tilde{W}_k Z_k - G_*)s_k\| \|G_*^{-1/2}\|]\right)$$
$$+4O(\|\alpha_k p_Y\|)^2,$$

and thus

$$\frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} \le 1 + O(\alpha_k) + \alpha_k O\left(\frac{\|p_Y\|}{\|s_k\|}\right) + \alpha_k O\left(\frac{\|\alpha_k p_Y\|^2}{\|s_k\|^2}\right). \tag{3.57}$$

The rest of the proof is identical to the one in our previous paper. We note from (2.15) that if BFGS updating of B_k takes place at iteration k, then $\|p_Y\| \le \gamma \|p_Z\|/\sigma_k^{1/2}$. Using this, (3.56) and the fact that G_k converges to zero, we see that for large k

$$\frac{\tilde{y}_k^T \tilde{s}_k}{\|\tilde{s}_k\|^2} = 1 + O(\sigma_k^{1/2}),$$

and using (3.57)

$$\frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} = 1 + O(\sigma_k^{1/2}).$$

Therefore

$$\frac{\|\tilde{y}_k\|^2 \; \|\tilde{s}_k\|^2}{\dots} \quad O(\sigma_k^{1/2}) \tag{3.58}$$

We now consider $\psi(\tilde{B}_{k+1})$ given by (3.38). Noting that $\ln(1 + O(\sigma_k^{1/2})) = O(\sigma_k^{1/2})$ for all large k, we see that if updating takes place at iteration k

$$\psi(\tilde{B}_{k+1}) = \psi(\tilde{B}_k) + O(\sigma_k^{1/2}) + \ln\cos^2\tilde{\theta}_k + \left[1 - \frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k} + \ln\frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k}\right]. \tag{3.59}$$

Since both $\ln\cos^2\tilde{\theta}_k$ as well as the term inside the square brackets are non-positive, we can delete them to obtain

$$\psi(\tilde{B}_{k+1}) \le \psi(\tilde{B}_k) + O(\sigma_k^{1/2}). \tag{3.60}$$

We now combine the results of Parts I and II of this proof. Let us subdivide the set of iterates U for which BFGS updating takes place into two subsets: U' corresponds to the iterates in which $\overline{w}_k$ is computed by Broyden's method, and U'' to the iterates in which finite differences are used. We also define $U'_k = U' \cap \{1,2,\ldots k\}$ and $U''_k = U'' \cap \{1,2,\ldots k\}$.

Summing over the set of iterates in U_k, using (3.54) and (3.60), and noting that $B_{j+1} = B_j$ for $j \notin U_k$, we have

$$\psi(\tilde{B}_{k+1}) \le \psi(\tilde{B}_1) + C_1 \sum_{j\in U_k''} \sigma_j^{1/2} + C_2 \sum_{j\in U'_k} \sigma_j + C_3 \sum_{j\in U'_k} \dots \tag{3.61}$$

for some constants $C_U C_2, C_3$. By (3.31) and since $|U_j''| \leq |Uj|$,

$$\mathrm{E}_{j\in U''} a)^{\prime 2} \wedge \mathrm{E}_{j\in U''} C^{1/2} r^{|U_j|/2}$$

$$\leq \sum_{jeu''} C^{1/2} r^{|U_j''|/2}$$

$$= \sum_{i=i}^{|u''|} C^{1/2} r^{i/2}$$

$$< 00.$$

Similarly

$$\mathrm{E}_{j\in U'} {}^{\circ} i < \infty,$$

and since {7*} is summable we conclude from (3.61) that *{xp($\tilde{B}$k)}* is bounded above. By (3.32) *tl>($\tilde{B}$k)* = SJLiCt"- ln^t)> where Zj are the eigenvalues of i?*, and it is easy to see that this implies that both Hi?*II and HB^^{1}!! are bounded.

To prove (3.45), we sum relations (3.53) and (3.59), recalling that a*, 7* and $o^{\wedge 1/9}$ are summable, to obtain

$$\psi(\tilde{B}_{k+1}) \leq C + \sum_{j\in U_k} \text{fin} \cos^2 \tilde{e}_k + \left[\mathrm{i} - \frac{\ll}{\cos\ k} + \ln \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} \right] \Big),$$

for some constant *C.* Since *ip($\tilde{B}$k+\)* > 0, and since both $\ln \cos^2 0^*$ and the term inside the square brackets are non-positive we see that

$$\lim_{\substack{k\to\infty \\ keu}} \ln \cos^2 \tilde{0}^* = 0,$$

and

$$\lim_{\substack{k\to\infty \\ k\in U}} \left[1 - \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} + \ln \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} \right] \to 0.$$

Now, for a; $\geq$ 0 the function $1 - x + \ln x$ is concave and has its unique maximizer at $x = 1$. Therefore the relations above imply that

$$\lim_{\substack{k\to\infty \\ k\in U}} \cos \mathrm{fj}^* = \lim_{\substack{k\to\infty \\ k\in U}} \tilde{g}^* = 1. \tag{3.62}$$

Now from (3.36)-(3.37)

$$\frac{\|G_*^{-1/2} B_k - G_*)p_z\|^2}{\|G_*^{1/2} p_z\|^2} = \frac{\|(\tilde{B}_k - I)\tilde{s}_k\|^2}{\|\tilde{s}_k\|^2}$$

$$= \frac{\|\tilde{B}_k \tilde{s}_k\|^2 - 2\mathrm{i}^{\wedge} \tilde{B}_k \tilde{s}_k + \tilde{s}_k^T \tilde{s}_k}{\tilde{s}_k^T \tilde{s}_k}$$

$$= \frac{\tilde{q}_k^2}{\cos 0f} - 2\tilde{q}_k + 1.$$

It is cleax from (3.62) that the last term converges to 0 for k 6 £/, which implies that (3.45) holds.

a

This result immediately implies that the iterates are R-linearly convergent, regardless of how often updating takes place.

Theorem 3.9 *Suppose that the iterates {x^} generated by Algorithm I converge to a solution point x+ that satisfies Assumptions 3.2. Then the rate of convergence is at least R'linear.*

Proof. Theorem 3.8 implies that the condition number of the matrices {£*} is bounded. Therefore *all* the iterates are good iterates, and reasoning as in the proof of Theorem 3.6 we conclude that for all j

$$\|x_j - x^*\| \leq C r^j,$$

for some constants $C > 0$ and $0 \leq r < 1$.

D

As in our previous paper, we also note that the Broyden matrices S* are bounded and this follows directly from R-linear convergence and the well-known bounded deterioration property for Broyden's method (cf. Lemma 8.2.1 in Dennis and Schnabel (1983)).

3.4. Superlinear Convergence

Without the correction terms W_k and x̄fik, and using appropriate update criteria, Algorithm I is 2-step Q-superlinearly convergent. This was proved by Nocedal and Overton (1985) assuming that Y* and Z_k are orthogonal bases, and that a good starting matrix B_1 is used. This result has been extended by Xie (1991) for more general bases and for any positive definite starting matrix B_1.

To establish 1-step superlinear convergence we need to assume that the steplengths α_k have the value 1 for all large A; When a smooth merit function, such as Fletcher's differentiable function (Fletcher (1973)) is used, it is not difficult to show that near the solution unit steplengths give a sufficient reduction in the merit function and will be accepted.

However the non-differentiable £\ merit function (1.7) used in this paper may reject steplengths of one, even though the lower bound on \i is weaker than ‖A‖oo« Thus the multiplier-free method can still suffer from the Maratos effect; the algorithm must be modified to allow unit steplengths and to achieve a fast rate of convergence. (In the numerical experiments described in the next section, we employ a non-monotone line search (or watchdog technique) of Chamberlain et al (1982) that allows unit steplengths to be accepted for all large fc. The analysis of the modified algorithm would be similar to that presented in §5.5 of Byrd and Nocedal (1991).)

Nevertheless, if we assume that the iterates generated by Algorithm I converge R-linearly to a solution and that unit steplengths are taken for all large fc, then the performance of the method is no longer influenced by the merit function and the analysis is identical to that of our previous paper. The convergence result can therefore be summarized by:

Theorem **3.10** *Suppose that the iterates generated by Algorithm I converge R-linearly to a point x+ that satisfies Assumptions 3.2, and that* a* = 1 *for all large k. Then the rate of convergence is 1-step Q-superlinear.*

4. *

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