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**Convergence Analysis for a Multiplier-Free
Reduced Hessian Method**

Lorenz T. Biegler

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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

$$\min_{x \in \mathbb{R}^n} f(x) \quad (1.1)$$

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

where $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $c : \mathbb{R}^n \rightarrow \mathbb{R}^m$ 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 k , a search direction d_k by solving

$$\min_{d \in \mathbb{R}^n} g(x_k)^T d + \frac{1}{2} d^T W(x_k) d \quad (1.3)$$

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

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

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

A new iterate is then computed as

$$x_{k+1} = x_k + a_k d_k \quad (1.6)$$

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 ℓ_1 merit function

$$\hat{f}(x) = f(x) + M \|c(x)\|_1, \quad (1.7)$$

where M 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 $(\hat{f}^{\wedge} x)$.

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

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

where $Y_k \in \mathbb{R}^{n \times m}$ and $Z_k \in \mathbb{R}^{n \times (n-m)}$, and assume that

$$A Z_k = 0. \quad (1.9)$$

(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

$$d_k = Y_k p_Y + Z_k p_Z \quad (1.10)$$

for some vectors $p_Y \in \mathbb{R}^m$ and $p_Z \in \mathbb{R}^{n-m}$. Due to (1.9) the linear constraints (1.4) become

$$c_k + A Y_k p_Y = 0. \quad (1.11)$$

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

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

Substituting this in (1.10) we have

$$d_k = -Y_k [A Y_k]^{-1} c_k + Z_k p_Z \quad (1.13)$$

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

$$\min_{p_Z \in \mathbb{R}^{n-m}} (Z_k^T g_k + Z_k^T W_k Y_k p_Y)^T p_Z + \frac{1}{2} p_Z^T (Z_k^T W_k Z_k) p_Z. \quad (1.14)$$

Assuming that $Z^T W_k Z_k$ is positive definite, the solution of (1.14) is

$$p_z = -(Z^T W_k Z_k)^{-1} (Z^T g_k + Z^T W_k Y_k p_Y). \quad (1.15)$$

This determines the search direction of the SQP method.

In our previous paper (Biegler, Nocedal and Schmid, 1995) the cross term $[Z^T W_k Y_k] p_Y$ is approximated by a vector w_k ,

$$[Z^T W_k Y_k] p_Y \approx w_k, \quad (1.16)$$

without computing the matrix $Z^T W_k Y_k$. 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

$$p_z = -\{Z^T W_k Z_k\}^{-1} [Z^T g_k + (w_k)], \quad (1.17)$$

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

Here the cross term is approximated either by a finite difference estimate along $Y_k p_Y$ or by a quasi-Newton method in which the rectangular matrix $Z^T W_k$ is approximated by a matrix S_k , using Broyden's method. We then obtain w_k by multiplying this matrix by $Y_k p_Y$, i.e.,

$$w_k = S_k Y_k p_Y.$$

In this study, we update S_{k+1} so that it satisfies the following secant relation:

$$S_{k+1}(x_{k+1} - x_k) = Z^T g_{k+1} - Z^T g(x_k). \quad (1.18)$$

Let us now consider how to approximate the reduced Hessian matrix $Z^T W_k Z_k$. From (1.6), (1.10) and (1.18) we obtain

$$[S_{k+1} Z_k] a_k p_z = -a_k S_{k+1} (Y_k p_Y) + Z^T g_{k+1} - Z^T g(x_k).$$

Since S_{k+1} approximates $Z^T W$, this suggests the following secant equation for $Z^T W$, the quasi-Newton approximation to the reduced Hessian $Z^T W Z$:

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

where s_k and y_k are defined by $s_k = a_k p_z$ and

$$y_k = Z^T g_{k+1} - Z^T g(x_k) - \bar{w}_k, \quad (1.20)$$

with

$$W_k = a_k S_M(Y_k p_Y). \quad (1.21)$$

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

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}, \quad (1.22)$$

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

$$B_k Pz = -\{Zk^T g_k + O(\epsilon)\} \quad (1.23)$$

Note as in our previous paper, that two correction terms, Wk and $\bar{W}k$ are applied. The first term, Wk , is used in the null space step (1.23) and makes use of the matrix S^* . The second term, $\bar{W}k$ is used in (1.20) for the BFGS update of Bk and is computed using the new Broyden matrix S_{fc+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:

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

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

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

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

$$Z(\hat{x})^T VL(\hat{x}; \bar{x}) = Z(\bar{x})^T g(\bar{x}) \quad (1.27)$$

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

$$\begin{aligned} Wk &= Z(\hat{x})^T VL(\hat{x}; \bar{x}) - Z(\bar{x})^T g(\bar{x}) \\ &= Z(\hat{x})^T VL(\hat{x}; \bar{x}) - Z(\bar{x})^T g(\bar{x}) - Wk \end{aligned} \quad (1.28)$$

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 α_k , and the procedure for updating the weight f_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 Z_k , and could be denoted by p_Y^k and p_z^k but we will normally omit the superscript for simplicity. The symbol $\|\cdot\|$ denotes the L_2 vector norm or the corresponding induced matrix norm. When using the L_1 or L_∞ norms we will indicate it explicitly by writing $\|\cdot\|_1$ or $\|\cdot\|_\infty$. A solution of problem (1.1) is denoted by x^* , and we define

$$e_k = x_k - x^* \quad \text{and} \quad a_k = \max\{\|e_k\|, \|e_{k+1}\|\}. \quad (1.29)$$

2. Details of the Multiplier-Free Algorithm

In this section we consider¹ how to calculate approximations w_k and \bar{w}_k to $(Z^T W_k Y_k) p_Y$ to be used in the determination of the search direction p_z and in updating x^* , respectively. We also discuss when to skip the BFGS update of the reduced Hessian approximation, as well as the selection of the damping factor C_k and the penalty parameter λ_k .

To approximate to $(Z^T W_k Y_k) p_Y$ we propose two approaches that have slight modifications to those proposed in our earlier paper. First, we consider a finite difference approximation to $Z^T W_k$ along the direction $Y_k p_Y$. The second approach defines w_k and \bar{w}_k in terms of a Broyden approximation to $Z^T W_k$, 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 \bar{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

$$w_k = Z(x_k + Y_k p_Y)^T g(x_k + Y_k p_Y) - Z^T g_k. \quad (2.1)$$

After the step to the new iterate x_{k+1} has been taken, we define

$$\bar{w}_k = a_k w_k \quad (2.2)$$

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

$$w_k = Z^T [VL(x_k + Y_k p_Y, X_k) - VL(x_k, X_k)]. \quad (2.3)$$

$$\bar{w}_k = Z^T [VL(x_k + a_k Y_k p_Y, X_M) - VL(x_k, X_{k+1})] \quad (2.4)$$

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

We can approximate the rectangular matrix $Z^T W_k$ by a matrix S_k^* updated by Broyden's method, and then compute w_k and \bar{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))

$$S_k = S_k + \frac{(f_{fc} - f_{fc}^*)}{s_k^T s_k} s_k \quad (2.5)$$

where

$$f_{fc} = Z_k^T f_{fc} - Z_k^T g(x_k) \quad (2.6)$$

$$s_k = Z_k^T f_{fc} - x_k \quad (2.7)$$

thus, defining

$$w_k = S_k Y_k p_Y \quad \text{and} \quad \bar{w}_k = a_k S_k + i Y_k p_Y \quad (2.8)$$

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

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

On the other hand, the correction \bar{w}_k will be safeguarded by choosing a sequence of positive numbers $\{\gamma_k\}$ such that $\sum \gamma_k < \infty$, and set

$$\bar{w}_k = \begin{cases} \bar{w}_k & \text{if } \|\bar{w}_k\| \leq \alpha_k \|p_Y\| / \gamma_k \\ \bar{w}_k \frac{\alpha_k \|p_Y\|}{\gamma_k \|\bar{w}_k\|} & \text{otherwise.} \end{cases} \quad (2.10)$$

As the iterates converge to the solution, $p_Y \rightarrow 0$, 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 $s^T y_k > 0$ 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 $s^T y_k > 0$ 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

$$\begin{aligned} y_k &= Z_k^T g_{fc} - \bar{w}_k \\ &= Z_{k+1}^T \nabla L(x_{k+1}, \lambda_*) - Z_k^T \nabla L(x_k, \lambda_*) - \bar{w}_k \\ &= Z_k^T \int_0^1 V_{xx} L(x_k + r a_k d_k, \lambda_*) dr \, a_k d_k + (Z_{fc} - Z_k)^T \nabla L(x_k + u_k) - \bar{w}_k \\ &\equiv Z_k^T \bar{w}_k a_k d_k + (Z_{fc} - Z_k)^T \nabla L(x_{fc}, \lambda_*) - \bar{w}_k \\ &= Z_k^T \bar{w}_k Z_k s_k + O(\alpha_k \|s_k\| + \alpha_k \|p_Y\|) + \alpha_k Z_k^T \bar{w}_k Y_k p_Y - \bar{w}_k, \end{aligned} \quad (2.11)$$

where we have defined

$$Z_k^T \tilde{W}_k = \int_{J_0}^1 V_{xx}^2 L(x_k + T a_k d_k, X.) dr. \quad (2.12)$$

Thus

$$s^T y_k = s^T_k \{ Z_k^T \tilde{W}_k Z_k \} s_k + O(a_k) \|s_k\| + [a_k s^T (Z_k^T W_k \tilde{Y}_k) p_Y - \#57^*] + O(o_k) \|a_k\| \|p_Y\|. \quad (2-13)$$

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

Update Criterion I.

Choose a constant $\gamma_{fd} > 0$ and a sequence of positive numbers $\{j_k\}$ such that $E_j \wedge^{\infty} < \infty$ (this is the same sequence $\{7^*\}$ that was used in (2.10)).

- If W_k is computed by Broyden's method, and if both $s^T y_k > 0$ and

$$\|b_{vll}\| \leq 7^{*2} IM \quad (2.14)$$

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

- If W_k is computed by finite differences, and if both $s^T y_k > 0$ and

$$\|p_Y\| \leq \gamma_{fd} \|p_Z\| / \sigma_1^{1/2} \quad (2.15)$$

hold at iteration k , then update the matrix B_k by means of the BFGS formula (1.22) with S_k and y_k given by (1.20). Otherwise, set $B_{k+i} = B_k$.

Here O_k 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 $(\|Z_{jj}^T\| + \|cfc\|)$. Moreover, define

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

From Byrd and Nocedal (1989), the behavior of $\cos \theta_k$ 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 $k \geq 1$, $S_k \wedge 0$ and

$$\frac{s_k^T s_k}{\|s_k\|^2} \geq m > 0 \quad (2.17)$$

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

Then, there exist constants $\beta_2, \beta_3 > 0$ such that, for any $k \geq 1$, the relations

$$\cos \theta_j \geq \beta_2 \tag{2.19}$$

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

hold for at least $\lfloor n/2 \rfloor$ values of $j \in [1, n]$.

This theorem refers to the iterates for which BFGS updating takes place, but since for the other iterates $B_{k+1} = \mathcal{E}^*$, the theorem characterizes the whole sequence of matrices $\{B_k\}$. Theorem 2.1 states that, if $s^T y^*$ 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 $\cos \theta_j$ is bounded away from zero and $B_j s_j = O(\|s_j\|)$. 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", and define $J_k = \{j \in [1, n] : j \in J\}$.

Note that if the matrices B_k are updated only a finite number of times, their condition number is bounded, and (2.19)-(2.20) are satisfied for all k . 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 $Z^T W Z$ is positive definite, then for all x_k in a neighborhood of x^* the smallest eigenvalue of $Z^T W Z$ is bounded away from zero (\bar{W} is defined in (2.12)). We now show that in such a neighborhood with ϵ sufficiently small that Update Criterion I implies (2.17)-(2.18). For the case when \bar{w} is computed by Broyden's method. Using (2.13), (2.14) and (2.10), and since γ^* converges to zero, we have

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

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

$$\begin{aligned}
 y_k &= Z_{k+1}^T g_{k+1} - Z_k^T g_k - \bar{w}_k \\
 &= Z_{k+1}^T \nabla L(x_{k+1}, \lambda_*) - Z_k^T \nabla \\
 &\quad L(x_k, A) - a_k [Z_{k+1}^T \nabla L(x_{k+1}, \lambda_*) - Z_k^T \nabla L(x_k + Y_k p_Y, A) - 2\% \nabla L(x_k, A)] \\
 &= (Z_{k+1}^T - Z_k^T) \nabla L(x_{k+1}, A) + Z_k^T (\nabla L(x_{k+1}, A) - \nabla L(x_k + Y_k p_Y, A)) \\
 &\quad - a_k [Z_{k+1}^T \nabla L(x_{k+1}, \lambda_*) - Z_k^T \nabla L(x_k + Y_k p_Y, A) \\
 &\quad + Z_k^T (\nabla L(x_k + Y_k p_Y, A) - \nabla L(x_k, A))] \\
 &= Z_k^T \tilde{W}_k Z_k s_k + a_k Z_k (\tilde{W}_k - \hat{W}_k) Y_k p_Y + O(a_k) \|s_k\| \\
 &= Z_k^T \tilde{W}_k Z_k s_k + O(a_k) \|s_k\|.
 \end{aligned}$$

assuming $Y_k p_Y = O(a_k)$. 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, $s^T y_k$ is sufficiently positive, as stipulated by (2.17)-(2.18).

2.4. A Multiplier-free Approach for Choosing n_k .

We will choose α so that for some $p > 0$,

$$\|M^H\| \geq \|A^* M^*\| + p \|c^*\| \quad (2.23)$$

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 λ merit function in the direction d^* is given by

$$D^{\lambda}(x_k; d_k) = g^T d_k - W^T d_k. \quad (2.24)$$

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

$$g(x)^T Y(x) p_Y = \lambda(x)^T c(x). \quad (2.25)$$

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

Theorem 2.1 Assume that $A(x)$ is of full column rank for all $x \in D$ and that $Z(x)$ is norm bounded. If $(p^{\lambda}(x))$ is defined by (1.7) and f^{λ} satisfies (2.23) for all $x \in D$, then $D^{\lambda}(x; d) > 0$ for all d satisfying $\tilde{c}(x) + A(x)^T d = 0$ if and only if x is a Kuhn-Tucker point.

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

$$\begin{aligned} 0 \leq D\phi_\mu(\bar{x}; d) &= \bar{g}(x) f d - n \|c(\bar{x})\| \beta \\ &= \bar{g}(\bar{x})^T Z(\bar{x}) p_z - \beta \|c(\bar{x})\| + X \bar{f}(\bar{x})^T c(\bar{x}) \\ &\leq \bar{g}(\bar{x})^T Z(\bar{x}) p_z - \beta \|c(\bar{x})\| \\ &\leq g(\bar{x})^T Z(\bar{x}) p_z \end{aligned} \quad (2.26)$$

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

$$\begin{aligned} 0 \leq Z^0(\bar{x}; d) &= \bar{f}(\bar{x})^T c(\bar{x}) - \beta \|c(\bar{x})\| \\ &\leq -\beta \|c(\bar{x})\| \\ &< 0. \end{aligned} \quad (2.27)$$

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

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

into the directional derivative:

$$\begin{aligned} D^{\wedge}(\bar{x}; \bar{c}) &= -g(\bar{x})^T Z(\bar{x}) p_z - \beta \|c(\bar{x})\| + (H\bar{x})^T c(\bar{x}) \\ &= 0. \end{aligned} \quad (2.29)$$

D

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

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

Now from (1.23) we have that

$$B_k S_k = -O L_k (Z_k^T g_k + \zeta_k w_k) \quad (2.31)$$

As shown in our previous paper,

$$\cos \theta_k = \frac{-(Z_k^T g_k + \zeta_k w_k)^T p_z}{\|2 \zeta_k w_k + \zeta_k w_k\| \|p_z\|} \quad (2.32)$$

If we satisfy the following property for f_i :

$$H_k \|c_k\| \geq \beta \|c_k\| + 2\beta \|c_k\| \quad (2.33)$$

or, equivalently, from (2.25):

$$\|w_k\| \geq \frac{\|g_k\|}{\|B_k\|} + 2\rho\|c_k\| \quad (2.34)$$

then substituting in (2.30), leads to:

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

Note also from (2.31) that

$$\frac{\|g_k\|}{\|B_k g_k\|} = \frac{\|g_k\|}{\|Z_k^T g_k + \zeta_k w_k\|}. \quad (2.36)$$

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

$$\frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\| \leq \|p_z^{(j)}\|, \quad \frac{1}{\beta_2} \|Z_j^T g_j + \zeta_j w_j\| \leq \|p_z^{(j)}\| \quad (2.37)$$

Using this and (2.19) in (2.35) we obtain, for $j \in J$,

$$\begin{aligned} D\phi_{\mu_j}(x_j; d_j) &\leq -\frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\|^2 \cos \theta_j - \zeta_j w_j^T p_z^{(j)} - 2\rho\|c_j\|_1 \\ &\leq -\frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\|^2 \cos \theta_j - \zeta_j w_j^T p_z^{(j)} - 2\rho\|c_j\|_1, \end{aligned}$$

where we have dropped the non-positive term $-\zeta_j w_j^T p_z^{(j)}$. Since we can assume that $\beta_3 > 1$ (it is defined as an upper bound in (2.20)), we have

$$D\phi_{\mu_j}(x_j; d_j) \leq -\frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\|^2 \cos \theta_j - 2\rho\|c_j\|_1$$

It is now clear that if

$$2C_j \cos \theta_j \|g_j + \zeta_j w_j\| - C_j w_j^T p_z^{(j)} \leq 2\rho\|c_j\|_1, \quad (2.38)$$

then for all $j \in J$,

$$D\phi_H(x_j; d_j) \leq -\frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\|^2 - 2\rho\|c_j\|_1. \quad (2.39)$$

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

We will choose β_3^* so that (2.38) holds for all iterations. To see how to do this we note from (1.23) that

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

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

$$Ck[2\cos\theta_k |g_k^T Z_k w_k| + w_k^T B^T Z_k g_k + Ck w_k^T B^T w_k] \leq \rho \|c_k\|_1. \quad (2.40)$$

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

$$\epsilon_k = \min\{1, C\hat{c}_k\} \quad (2.41)$$

where \hat{c}_k is the largest value that satisfies (2.40) as an equality.

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

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

Note that for $c_k = 0$, $\hat{c}_k = 0$ and thus μ_k is only updated when $c_k \neq 0$.

The damping factor ϵ_k^* and the updating formula for the penalty parameter μ_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 ϵ_k we have in particular

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

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

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

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 $\epsilon \in (0, 1/2)$, $p > 0$ and r, r' 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 $\{\tau_k\}$. Set $k := 1$ and choose a starting point x_i , an initial value $\lambda > 0$ for the penalty parameter, an $(n - m) \times (n - m)$ symmetric and positive definite starting matrix B and an $(n - m) \times n$ starting matrix S .

2. Evaluate λ_k, τ_k, c^* and A_k , and compute p_Y and Z^* .

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

$$(A_k Y_k) p_Y = -c^*. \quad (\text{range space step}) \quad (2.44)$$

4. Calculate u_k^* 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

$$B_k p_z = -\tau_k \bar{g}_k + C_k W_k \quad (\text{null space step}) \quad (2.45)$$

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

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

8. Define the search direction by

$$d_k = Y_k p_Y + Z_k p_z \quad (2.46)$$

and set $\alpha = 1$.

9. Test the line search condition

$$\langle \nabla f(x_k + \alpha d_k) | d_k \rangle \leq \langle \nabla f(x_k) | d_k \rangle + \alpha \lambda C_k \|\nabla f(x_k)\|. \quad (2.47)$$

10. If (2.47) is not satisfied, choose a new $\alpha \in [r \alpha, r' \alpha]$ and go to 9; otherwise set

$$x_{k+1} = x_k + \alpha d_k \quad (2.48)$$

11. Evaluate $\lambda_{k+1}, \tau_{k+1}, c_{k+1}^*$, A_{k+1} , and compute Y_{k+1} and Z_{k+1} .

12. Update λ_k so as to satisfy (2.42).

13. Update λ_{k+1} using equations (2.5) to (2.7). If $findiff = false$ calculate u_{k+1}^* by Broyden's method through equations (2.8) and (2.10); otherwise calculate W_{k+1} by (2.2).

14. If $s^k y_k \leq 0$ or if (2.15) is not satisfied, set $B^{k+1} = B_k$. Else, compute

$$s^k = -P_k z^k, \quad (2.49)$$

$$V_k = Z(x_k + s^k) - Z(x_k) - \bar{w}_k, \quad (2.50)$$

and compute B_{k+1} by the BFGS formula (1.22).

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

3. Convergence Results

In this section we summarize several convergence results for Algorithm I. Many of the results of 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 $\langle f \rangle^*$ 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 $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $c : \mathbb{R}^n \rightarrow \mathbb{R}^m$ and their first and second derivatives are uniformly bounded in norm over D .
- (II) The matrix $A(x)$ has full column rank for all $x \in D$, and there exist constants γ_0 and γ_1 such that

$$\gamma_0 \|A(x)\| \leq \|A(x)z\| \leq \gamma_1 \|z\|, \quad \|Z(s)\| \leq \gamma_2 \|s\|, \quad (3.1)$$

for all $x \in D$.

- (III) For all $k \geq 1$ for which B_k is updated, (2.17) and (2.18) hold.
- (IV) The correction term t^k is chosen so that there is a constant $K > 0$ such that for all

$$\|w_k\| \leq K \|t^k\|^2. \quad (3.2)$$

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 $\|g_j\| = \beta_j$, is constant for all sufficiently large j , then there is a positive constant γ such that for all large $j \in J$,

$$\phi_\mu(x_j) - \phi_\mu(x_{j+1}) \geq \gamma M [\|g_j\|^2 + \|c_j\|]. \quad (3.3)$$

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 $\{\beta_k\}$ are constant for all sufficiently large k and $\lim_{k \rightarrow \infty} (\|Z_k^T g_k\| + \|c_k\|) = 0$.

Proof. First note that by Assumptions 3.1 (I)-(II) and (2.25) that $\{\|Z_k^T p_k\| / \|c_k\|\} = \{\|f_k\| / \|c_k\|\} \wedge \{1/\beta_k\}$ is bounded. Therefore, since the procedure (2.42) increases β_k by at least p whenever it changes the penalty parameter, it follows that there is an index k_0 and a value β such that for all $k > k_0$, $\beta_k \geq \beta \|c_k\| + 2p \|c_k\| \beta_j$. 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 $\langle f \rangle_n(x_k)$ decreases at each iterate, we have that for $k \in J$,

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

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

$$\lim_{j \in J} (\|Z_j^T g_j\|^2 + \|c_j\|) = 0. \quad (3.4)$$

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

$$\lim (\|Z_j^T g_j\|^2 + \|c_j\|) = 0.$$

□

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 β^* is chosen large enough, then x^*

is a point of attraction for the sequence of iterates $\{x_k\}$ 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.

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

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

(1) The functions $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $c : \mathbb{R}^n \rightarrow \mathbb{R}^m$ are 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 $A^* \in \mathbb{R}^m$ such that

$$V_L(z^*, A^*) = g(x_m) + A^* \lambda^* = 0.$$

(3) For all $q \in \mathbb{R}^{n-m}$, $q^T G^* q > 0$.

(4) There exist constants γ_0, γ_1 and γ_C such that, for all x in a neighborhood of x^* ,

$$\|Y(x)Z(x)\| \leq \gamma_0, \quad \|Z(x)\| \leq \gamma_1, \quad (3.6)$$

and

$$\|Y(x)Z(x)\| \leq \gamma_C. \quad (3.7)$$

(5) $Z(x)$ and $Y(x)$ are Lipschitz continuous in a neighborhood of x^* , i.e. there exist constants γ_z and γ^* such that

$$\|\lambda(x) - \lambda(z)\| \leq \gamma_\lambda \|x - z\|, \quad (3.8)$$

$$\|Z(x) - Z(z)\| \leq \gamma_z \|x - z\|, \quad (3.9)$$

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 $q \in \mathbb{R}^{n-m}$,

$$m\|q\|^2 \leq q^T G(x) q \leq M\|q\|^2, \quad (3.10)$$

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^*

$$\|Z(x)^T g(x)\| \leq \|c(x)\| + \gamma_2 \|x - x^*\|, \quad (3.11)$$

for some positive constants γ_1, γ_2 .

This result states that, near x^* , 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 $\gamma_3 > 0$ and $\gamma_4 > 0$, such that for all x sufficiently near x^*

$$\|Z(x)^T g(x)\|^2 \leq M^x \sim M^{x''} \leq \gamma_4 (\|Z(x)^T g(x)\|^2 + \|c(x)\|). \quad (3.12)$$

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

$$\|Z(x)^T g(x)\| = \|Z(x)^T \nabla L(x, \lambda^*)\| \quad (3.13)$$

$$= \|Z(x)^T \nabla L(x, \lambda^*) - Z(x)^T \nabla L(x, \lambda^*)\| \quad (3.14)$$

$$\geq L(x, \lambda^*) + \lambda^* \nabla L(x, \lambda^*) - \lambda^* \nabla L(x, \lambda^*) \quad (3.15)$$

$$\geq L(x, \lambda^*) + \|c(x)\| \quad (3.16)$$

$$(3.17)$$

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

$$\begin{aligned} \phi_\mu(x) - \phi_\mu(x^*) &\geq \nabla L(x^*, \lambda^*)^T (x - x^*) + \frac{1}{2} (x - x^*)^T \nabla_{xx}^2 L(x^*, \lambda^*) (x - x^*) \\ &\quad + \gamma \|c(x)\|_1 + \gamma \|c(x)\|^2 - \gamma \|c(x)\|^2 + O(\|x - x^*\|^3) \end{aligned} \quad (3.18)$$

Now we note that

$$\nabla_{xx}^2 L(x, \lambda^*) = \nabla_{xx}^2 L(x^*, \lambda^*) + O(\|x - x^*\|). \quad (3.19)$$

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 ν such that:

$$\nu \nabla_{xx}^2 L(x, \lambda^*) + \nu \nabla_{xx}^2 L(x^*, \lambda^*) (x - x^*) \geq 2\gamma_3 \|a; -x, f\| \quad (3.20)$$

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

$$\phi_\mu(x) - \phi_\mu(x^*) \geq 2\gamma_3 \|x - x^*\|^2 + \gamma \|c(x)\|_1 + O(\|x - x^*\|^3) \quad (3.21)$$

$$\geq 731k \cdot ar \cdot \|x - x^*\|^2 \quad (3.22)$$

$$(3.23)$$

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

$$M(x) - \frac{1}{2} \|c(x)\|_1^2 = \frac{1}{2} L(x, A) - f(x) + \frac{1}{2} \|c(x)\|_1^2 \quad (3.24)$$

$$= \frac{1}{2} L(x, A) - f(x) + \frac{1}{2} \|c(x)\|_1^2 \quad (3.25)$$

$$\leq O(\|x - x^*\|^2) + p \|c(x)\|_1 \quad (3.26)$$

$$\leq \gamma_4 [\|Z(x)^T g(x)\|^2 + \|c(x)\|_1] \quad (3.27)$$

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 , $\langle (1 - \theta)x_k + \theta x_{k+1} \rangle \in \{x : \langle \nabla M(x) \rangle \leq p \|c(x)\|_1\}$ 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 x_{k_0} is sufficiently close to a solution point x^* that satisfies Assumptions 3.2, and if the weight β_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 $\{\|A^k c\|\}$ is bounded. Therefore the procedure (2.42) ensures that the weights β_k are constant, say $\beta_k = \beta_0$ for all large k . 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 β_0 , 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 $\epsilon > 0$, there is an iterate x_{k_0} such that

$$\|x_{k_0} - x^*\| \leq \frac{\gamma_3}{\gamma_2 \gamma_4 \beta_0} \epsilon^2,$$

where β_0 is such that $\|\cdot\|_1 \leq \beta_0 \|\cdot\|_2$. Assumption 3.3 shows that for any $k \geq k_0$, x^* is in the connected component of the level set of x_{k_0} that contains x_{k_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) $\|x_k - x_*$ $\leq \gamma_3^{-\frac{1}{2}} (\phi_\mu(x_k) - \phi_\mu(x_*))^{1/2}$ for $k \geq k_0$, and since we can assume that $\|Z_{k_0}^T g_{k_0}\|^2 + \|c_{k_0}\|_1 \leq 1$ we have from Lemmas 3.3 and 3.4, for any $k \geq k_0$

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

This implies that the whole sequence of iterates remains in a neighborhood of radius ϵ of x_* . If ϵ is small enough we conclude by (3.12), by the monotonicity of $\{\phi_\mu(x_k)\}$ 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 $p > 0$, $\|x_k - x_*\| \leq p \|x_{k-1} - x_*\|$ and

$$\|c(x_k)\| \leq p \|c(x_{k-1})\| + M \|x_k - x_{k-1}\| \quad (3.28)$$

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,

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

and let

$$U_k = \{j \in U : j \geq k\}. \quad (3.30)$$

The number of elements in U_k will be denoted by $|U_k|$. 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 $k \in U$ and any $j \geq k$*

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

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

This result implies that if $\{U_k/k\}$ is bounded away from zero, then Algorithm I is R-linearly 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 $\{U_k/k\} \rightarrow 0$. We therefore need to examine the iteration more closely.

We make use of the matrix function ψ defined by

$$\psi(B) = \text{tr}(B) - \ln(\det(B)), \quad (3.32)$$

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

$$\text{Incond}(B) < V > (\epsilon), \quad (3.33)$$

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

$$Vk = G^{1/2} y_k, \quad \tilde{s}_k = G^T J^2 s_k, \quad (3.34)$$

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

$$\cos \tilde{\theta}_k = \frac{\tilde{s}_k^T \tilde{B}_k \tilde{s}_k}{\|\tilde{s}_k\| \|\tilde{B}_k \tilde{s}_k\|}, \quad (3.36)$$

and

$$\tilde{q}_k = 2 \frac{G \wedge s_k}{s_k} \quad (3.37)$$

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

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

This expression characterizes the behavior of the BFGS matrices B_{k_j} 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 are used to estimate w_k and TU^A , these are accurate to second order.

Lemma 3.7 // at the iterate x_k , the corrections w_k and \tilde{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

$$\|\tilde{w}_k\| = O(\|b_k\|), \quad (3.39)$$

$$\|K - Z;^T W; y_{fc} p_Y\| = O(\alpha_k \|p_Y\|). \quad (3.40)$$

and

$$\|\tilde{w}_k - \alpha_k Z^T W; Y_k p_Y\| = O(\sigma_k \|p_Y\|). \quad (3.41)$$

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

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

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

$$VL(x_k + Y_k p_Y, A) = O(\|x - x_m\|) + O(\|b_Y\|) = O(a_k) \tag{3.43}$$

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

$$[Z_k^T \bar{W}_k - Z_k^T W_k] Y_k p_Y = O(\|b_Y\|) \|p_Y\| \tag{3.44}$$

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 $\{\|B^k\|\}$ and $\{\|B^k\|^{-1}\}$ are bounded, and for all $k \in U$*

$$\|(B_k - Z_k^T \bar{W}_k) p_Z\| = o(\|d_k\|). \tag{3.45}$$

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 B_k takes place. We have from (2.50), (2.48), (2.46), (2.12) and (2.49)

$$\begin{aligned}
y_k &= Z_{k+1}^T g_{k+1} - Z_k^T g_k - \bar{w}_k \\
&= Z_{k+1}^T \nabla L(x_{k+1}, X) - Z_k^T [VL(x_k, X) - \bar{w}_k] \\
&= (Z_{k+1} - Z_k)^T VL(x_{k+1}, A) + Z_{k+1}^T VL(x_{k+1}, A) - VL(x_k, A) - \bar{w}_k \\
&= (Z_{k+1} - Z_k)^T VL(x_{k+1}, A) + [Z_{k+1}^T \int_0^1 V_{xx}^2 L(x_k + T a_k d_k, A) r dr] a_k d_k - \bar{w}_k \\
&= c_{T_k} Z_k^T \bar{W}_k (Z_k p_Z + Y_k p_Y) - \bar{w}_k + O(\tau_{fc} (\|a_k\| + a_k \|p_Y\|)) \\
&= Z_k^T \bar{W}_k Z_k p_Z + a_k [Z_k^T \bar{W}_k - Z_k^T W_k] Y_k p_Y + (a_k Z_k^T W_k Y_k p_Y - \bar{w}_k) \\
&\quad + O(a_k (\|s_k\| + a_k \|p_Y\|)).
\end{aligned} \tag{3.46}$$

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 $\|Z\|\bar{W}_k - Z_j W_{fc}\| = O(o_k)$, and from (2.10) we have that $\bar{w}_k = O(\|p_Y\|/7fc)$. Using this and Assumptions 3.2 in (3.46) we have

$$\begin{aligned} y_k &= Z\bar{W}_k Z_k s_k + \{a_k + l + 1/7^*\}O(a^*\|p_Y\|) + O(a_k)\|s_k\| \\ &= (Z\bar{W}_k Z_k - G_*)s_k + G_* s_k + (a^* + 1 + 1/\gamma_k)O(\alpha_k\|p_Y\|) + O(\sigma_k)\|s_k\| \end{aligned} \quad (3.47)$$

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

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

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

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

Similarly from (3.47) and (3.34) we have

$$\begin{aligned} \tilde{y}_k^T \tilde{y}_k &\leq \|(Z_k^T \bar{W}_k Z_k - G_*)s_k\|^2 \|G_*^{-1}\| \\ &\quad + 2(1 + O(a_k))\|(Z\bar{W}_k Z_k - G_*)s_k\| \|G_*^{1/2}\| \|s_k\| + (l + O(a_{fc}))^2 \|s_k\|^2 \\ &\quad + 2(\sigma_k + 1 + 1/\gamma_k)O(\|\alpha_k p_Y\|)\|G_*\| (\|s_k\| + \|2\bar{W}_k Z_k - G_*\| \|s_k\| \|G_*^{-1/2}\|) \\ &\quad + (\sigma_k + 1 + 1/\gamma_k)^2 O(\|\alpha_k p_Y\|)^2, \end{aligned} \quad (3.49)$$

and thus

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

At this point we invoke the update criterion, and note from (2.14) that if BFGS updating of B_k takes place at iteration fc , then $\|afcp_Y\| \leq 7fc\|sfc\|$ where $\{7^*\}$ is summable. Using this, the assumption that o_k converges to zero, and (3.48) we see that for large k

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

and using (3.50)

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

Therefore

$$\frac{\|\tilde{y}_k\|^2}{\tilde{y}_k \tilde{s}_k} = \frac{\|\tilde{y}_k\|^2 \|\tilde{s}_k\|^2}{\|\tilde{s}_k\|^2 \tilde{y}_k \tilde{s}_k} = 1 + O(\sigma_k + \gamma_k). \quad (3.52)$$

We now consider $x > \tilde{B}_k + i$ given by (3.38). A simple expansion shows that for large \tilde{y}_k , $\ln(1 + O(a_k + 7_{fc})) = O(a_k + 7_{fc})$. Using this, (3.51) and (3.52) we have

$$4 > \tilde{B}_M = 1 > \tilde{B}_k + O(a_k + 7_{fc}) + \ln \cos^2 \tilde{\theta}_k + \left[1 - \frac{1}{\cos^2 \tilde{\theta}_k} - \ln \frac{1}{\cos^2 \tilde{\theta}_k} \right]. \quad (3.53)$$

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

$$iK\tilde{B}_M < a_k + 7_{fc} + O(a_k + 7_{fc}). \quad (3.54)$$

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 \tilde{w}_k is computed by finite differences. In this case (2.15) holds. Again we begin by considering (3.46),

$$y_k = Z_k^{-1} \tilde{W}_k^{-1} (Z_k^{-1} \tilde{W}_k^{-1} + a_k \tilde{W}_k^{-1} - Z_k^{-1} \tilde{W}_k^{-1}) Y_k p_Y + (\alpha_k Z_k^{-1} \tilde{W}_k^{-1} Y_k p_Y - \tilde{w}_k) + O(\sigma_k)(\|s_k\| + \alpha_k \|p_Y\|).$$

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

$$\begin{aligned} y_k &= Z_k^{-1} \tilde{W}_k^{-1} Z_k s_k + O(\sigma_k)(\|s_k\| + \alpha_k \|p_Y\|) \\ &= \{Z_k^{-1} \tilde{W}_k^{-1} Z_k - G_k\} s_k + G_k s_k + O(a_k)(\|s_k\| + a_k \|p_Y\|). \end{aligned} \quad (3.55)$$

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

$$\tilde{y}_k \tilde{s}_k = s_k \{Z_k^{-1} \tilde{W}_k^{-1} Z_k - G_k\} s_k + \|h\|^2 + O(a_k)(\|s_k\|^2 + \alpha_k \|p_Y\| \|s_k\|),$$

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

$$\begin{aligned} \frac{\tilde{y}_k \tilde{s}_k}{\tilde{y}_k \tilde{s}_k} &= 1 + \frac{s_k^T \{Z_k^{-1} \tilde{W}_k^{-1} Z_k - G_k\} s_k}{\|s_k\|^2} + O(a_k) \left(1 + \frac{\alpha_k \|p_Y\|}{\|s_k\|} \right) \\ &= 1 + O(\sigma_k) + O\left(\sigma_k \frac{\alpha_k \|p_Y\|}{\|s_k\|}\right). \end{aligned} \quad (3.56)$$

Similarly from (3.55) and (3.34) we have

$$\begin{aligned} \tilde{y}_k^T \tilde{y}_k &< \|\tilde{Z}_k^T \tilde{W}_k \tilde{Z}_k - G_k\|_{S_k} \|\tilde{G}_k\| \\ &+ 2(1 + O(a_k)) \|\tilde{Z}_k^T \tilde{W}_k \tilde{Z}_k - G_k\|_{S_k} \|\tilde{G}_k\|^{1/2} \|\mathbf{p}^*\| + (1 + O(a_k)) \|\tilde{s}_k\|^2 \\ &+ \sigma_k O\left(\|\alpha_k \mathbf{p}_Y\| \|\tilde{G}_k\|^{-1/2} \left[\|(1 + O(a_k)) \|\tilde{s}_k\| + \|(Z_k^T \tilde{W}_k Z_k - G_k)_{S_k}\| \|\tilde{G}_k\|^{-1/2}\|\right]\right) \\ &+ 4O(\|a_{kPY}\|)^2, \end{aligned}$$

and thus

$$\frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} < 1 + O(a_k) + \frac{a_k O(\|\mathbf{p}_Y\|)}{\|\tilde{s}_k\|} + o\left(\frac{\|\alpha_k \mathbf{p}_Y\|^2}{\|\tilde{s}_k\|^2}\right). \quad (3.57)$$

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 $\|\mathbf{p}_Y\| \leq 7fd\|Pz\|/cric^2$. 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

$$\|\tilde{y}_k\|^2 \|\tilde{s}_k\|^2 = n(n-1/2) \|\tilde{s}_k\|^4$$

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

$$\psi(\tilde{B}_{k+1}) = \psi(\tilde{B}_k) + O(a_k^{1/2}) + \ln \cos^2 \theta_k + \ln \frac{1 - \cos^2 \theta_k}{\cos^2 \theta_k} + \ln \frac{1 - \cos^2 \theta_k}{\cos^2 \theta_k}. \quad (3.59)$$

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

$$\psi(\tilde{B}_{k+1}) < \psi(\tilde{B}_k) + O(a_k^{1/2}). \quad (3.60)$$

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^I corresponds to the iterates in which \tilde{w}_k is computed by Broyden's method, and U^II to the iterates in which finite differences are used. We also define $U^I_k = U^I \cap \{1, 2, \dots, A\}$ and $U^II_k = U^II \cap \{1, 2, \dots, fc\}$.

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

$$\psi(\tilde{B}_{k+1}) \leq \psi(\tilde{B}_1) + C_1 \sum_{j \in U^I_k} a_j^{1/2} + C_2 \sum_{j \in U^II_k} Y_j + C_3 \sum_{j \in U^II_k} \xi_j \quad (3.61)$$

for some constants C_1, C_2, C_3 . By (3.31) and since $|U_j'| \leq |U_j|$,

$$\begin{aligned} \mathbf{E}^a)^{1/2} \wedge \mathbf{E} & \sum_{j \in U''} C^{1/2} \tau^{1/2} |U_j|^{1/2} \\ & \leq \sum_{j \in U''} C^{1/2} \tau^{1/2} |U_j'|^{1/2} \\ & = \sum_{i=1}^{|U''|} C^{1/2} \tau^{1/2} \\ & < \infty. \end{aligned}$$

Similarly

$$\mathbf{E} \bullet j < \infty,$$

and since $\{7^*\}$ is summable we conclude from (3.61) that $\{xp(\bar{B}_k)\}$ is bounded above. By (3.32) $\langle \bar{B}_k \rangle = \text{SJLiCt}'' - \ln \langle \bar{B}_k \rangle$ where Z_j are the eigenvalues of i^* , and it is easy to see that this implies that both $\text{H}^* \Pi$ and $\text{H} \bar{B}^{\wedge 1}$ are bounded.

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

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

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

$$\lim_{k \rightarrow \infty} \ln \cos^2 \bar{\theta}_k = 0,$$

and

$$\lim_{k \rightarrow \infty} \left[1 - \frac{\bar{q}_k}{\cos^2 \bar{\theta}_k} + \ln \frac{\bar{q}_k}{\cos^2 \bar{\theta}_k} \right] \rightarrow 0.$$

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

$$\lim_{k \rightarrow \infty} \cos^2 \bar{e}_k = \lim_{k \rightarrow \infty} \bar{g}_k = 1. \quad (3.62)$$

Now from (3.36)-(3.37)

$$\begin{aligned} \frac{\|G^{\wedge 1/2} (B_k - G) p_z\|^2}{\|G^{\wedge 1/2} p_z\|^2} & = \frac{\|(\bar{B}_k - I) \bar{s}_k\|^2}{\|\bar{s}_k\|^2} \\ & = \frac{\|\bar{B}_k \bar{s}_k\|^2 - 2i \wedge \bar{B}_k \bar{s}_k + \bar{s}_k^T \bar{s}_k}{\bar{s}_k^T \bar{s}_k} \\ & = \frac{\bar{q}_k^2}{\cos^2 \bar{\theta}_k} - 2\bar{q}_k + 1. \end{aligned}$$

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**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

$$\min_{x \in \mathbb{R}^n} f(x) \quad (1.1)$$

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

where $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $c : \mathbb{R}^n \rightarrow \mathbb{R}^m$ 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 k , a search direction d_k by solving

$$\min_{d \in \mathbb{R}^n} g(x_k)^T d + \frac{1}{2} d^T W(x_k) d \quad (1.3)$$

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

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

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

A new iterate is then computed as

$$x_{k+1} = x_k + a_k d_k \quad (1.6)$$

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 ℓ_1 merit function

$$\hat{f}(x) = f(x) + M \|c(x)\|_1, \quad (1.7)$$

where M 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 $\hat{f}(x)$.

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

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

where $Y_k \in \mathbb{R}^{n \times m}$ and $Z_k \in \mathbb{R}^{n \times (n-m)}$, and assume that

$$AZ_k = 0. \quad (1.9)$$

(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

$$d_k = Y_k p_Y + Z_k p_Z \quad (1.10)$$

for some vectors $p_Y \in \mathbb{R}^m$ and $p_Z \in \mathbb{R}^{n-m}$. Due to (1.9) the linear constraints (1.4) become

$$c_k + AY_k p_Y = 0. \quad (1.11)$$

If we assume that A_k has full column rank then the nonsingularity of $[Y_k Z_k]$ and equation (1.9) imply that the matrix $A^T Y_k$ is nonsingular, so that p_Y is determined by (1.11):

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

Substituting this in (1.10) we have

$$d_k = -Y_k [A_k^T Y_k]^{-1} c_k + Z_k p_Z \quad (1.13)$$

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

$$\min_{p_Z \in \mathbb{R}^{n-m}} (Z_k^T g_k + Z_k^T W_k Y_k p_Y)^T p_Z + \frac{1}{2} p_Z^T (Z_k^T W_k Z_k) p_Z \quad (1.14)$$

Assuming that $Z^T W_k Z_k$ is positive definite, the solution of (1.14) is

$$p_z = -(Z^T W_k Z_k)^{-1} (Z^T g_k + Z^T W_k Y_k p_Y). \quad (1.15)$$

This determines the search direction of the SQP method.

In our previous paper (Biegler, Nocedal and Schmid, 1995) the cross term $[Z^T W_k Y_k] p_Y$ is approximated by a vector w_k ,

$$[Z^T W_k Y_k] p_Y \approx w_k, \quad (1.16)$$

without computing the matrix $Z^T W_k Y_k$. 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

$$p_z = -\{Z^T W_k Z_k\}^{-1} [Z^T g_k + (w_k)], \quad (1.17)$$

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

Here the cross term is approximated either by a finite difference estimate along $Y_k p_Y$ or by a quasi-Newton method in which the rectangular matrix $Z^T W_k$ is approximated by a matrix S_k , using Broyden's method. We then obtain w_k by multiplying this matrix by $Y_k p_Y$, i.e.,

$$w_k = S_k Y_k p_Y.$$

In this study, we update S_{k+1} so that it satisfies the following secant relation:

$$S_{k+1}(x_{k+1} - x_k) = Z^T g_{k+1} - Z^T g(x_k). \quad (1.18)$$

Let us now consider how to approximate the reduced Hessian matrix $Z^T W_k Z_k$. From (1.6), (1.10) and (1.18) we obtain

$$[S_{k+1} Z_k] a_k p_z = -a_k S_{k+1} (Y_k p_Y) + Z^T g_{k+1} - Z^T g(x_k).$$

Since S_{k+1} approximates $Z^T W$, this suggests the following secant equation for $Z^T W$, the quasi-Newton approximation to the reduced Hessian $Z^T W Z$:

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

where s_k and y_k are defined by $s_k = a_k p_z$ and

$$y_k = Z^T g_{k+1} - Z^T g(x_k) - \bar{w}_k, \quad (1.20)$$

with

$$W_k = a_k S_M(Y_k p_Y). \quad (1.21)$$

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

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}, \quad (1.22)$$

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

$$B_k Pz = -\{Zk^T g_k + O(\epsilon)\} \quad (1.23)$$

Note as in our previous paper, that two correction terms, Wk and $\bar{W}k$ are applied. The first term, Wk , is used in the null space step (1.23) and makes use of the matrix S^* . The second term, $\bar{W}k$ is used in (1.20) for the BFGS update of Bk and is computed using the new Broyden matrix S_{fc+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:

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

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

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

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

$$Z(\hat{x})^T VL(\hat{x}; \bar{x}) = Z(\bar{x})^T g(\bar{x}) \quad (1.27)$$

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

$$\begin{aligned} Wk &= Z(\hat{x})^T VL(\hat{x}; \bar{x}) - Z(\bar{x})^T g(\bar{x}) \\ &= Z(\hat{x})^T VL(\hat{x}; \bar{x}) - Z(\bar{x})^T g(\bar{x}) - Wk \end{aligned} \quad (1.28)$$

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 α_k , and the procedure for updating the weight f_i 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 Z_k , and could be denoted by p_Y^k and p_z^k but we will normally omit the superscript for simplicity. The symbol $\|\cdot\|$ denotes the L_2 vector norm or the corresponding induced matrix norm. When using the L_1 or L_∞ norms we will indicate it explicitly by writing $\|\cdot\|_1$ or $\|\cdot\|_\infty$. A solution of problem (1.1) is denoted by x^* , and we define

$$e_k = x_k - x^* \quad \text{and} \quad a_k = \max\{\|e_k\|, \|e_{k+1}\|\}. \quad (1.29)$$

2. Details of the Multiplier-Free Algorithm

In this section we consider¹ how to calculate approximations w_k and \bar{w}_k to $(Z^T W_k Y_k) p_Y$ to be used in the determination of the search direction p_z and in updating x^* , respectively. We also discuss when to skip the BFGS update of the reduced Hessian approximation, as well as the selection of the damping factor C_k and the penalty parameter λ_k .

To approximate to $(Z^T W_k Y_k) p_Y$ we propose two approaches that have slight modifications to those proposed in our earlier paper. First, we consider a finite difference approximation to $Z^T W_k$ along the direction $Y_k p_Y$. The second approach defines w_k and \bar{w}_k in terms of a Broyden approximation to $Z^T W_k$, 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 \bar{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

$$w_k = Z(x_k + Y_k p_Y)^T g(x_k + Y_k p_Y) - Z^T g_k. \quad (2.1)$$

After the step to the new iterate x_{k+1} has been taken, we define

$$\bar{w}_k = a_k w_k \quad (2.2)$$

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

$$w_k = Z^T [VL(x_k + Y_k p_Y, X_k) - VL(x_k, X_k)]. \quad (2.3)$$

$$\bar{w}_k = Z^T [VL(x_k + a_k Y_k p_Y, X_M) - VL(x_k, X_{k+1})] \quad (2.4)$$

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

We can approximate the rectangular matrix $Z^T W_k$ by a matrix S_k^* updated by Broyden's method, and then compute w_k and \bar{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))

$$S_k = Z_k^{-1} \left(g_k + \frac{(f_k - f(x_k)) \nabla f(x_k)}{s_k^T \nabla f(x_k)} \right) \quad (2.5)$$

where

$$Z_k = Z_k^{-1} (f(x_k) - f(x_{k-1})) - Z_{k-1} g_{k-1} \quad (2.6)$$

$$s_k = Z_k^{-1} (f(x_k) - f(x_{k-1})) - x_k \quad (2.7)$$

thus, defining

$$w_k = S_k Y_k p_Y \quad \text{and} \quad \bar{w}_k = a_k S_k + i Y_k p_Y \quad (2.8)$$

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

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

On the other hand, the correction \bar{w}_k will be safeguarded by choosing a sequence of positive numbers $\{\gamma_k\}$ such that $\sum \gamma_k < \infty$, and set

$$\bar{w}_k = \begin{cases} \bar{w}_k & \text{if } \|\bar{w}_k\| \leq \alpha_k \|p_Y\| / \gamma_k \\ \bar{w}_k \frac{\alpha_k \|p_Y\|}{\gamma_k \|\bar{w}_k\|} & \text{otherwise.} \end{cases} \quad (2.10)$$

As the iterates converge to the solution, $p_Y \rightarrow 0$, 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 $s^T y_k > 0$ 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 $s^T y_k > 0$ 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

$$\begin{aligned} y_k &= Z_k^{-1} (g_k - \bar{w}_k) \\ &= Z_{k+1}^{-1} \nabla L(x_{k+1}, \lambda_*) - Z_k^{-1} \nabla L(x_k, \lambda_*) - \bar{w}_k \\ &= Z_k^{-1} \int_0^1 V_{xx} L(x_k + r a_k d_k, \lambda_*) dr \int_0^1 a_k d_k + (Z_{k+1}^{-1} - Z_k^{-1})^T \nabla L(x_k + u a_k d_k, \lambda_*) - \bar{w}_k \\ &\equiv Z_k^{-1} \bar{w}_k a_k d_k + (Z_{k+1}^{-1} - Z_k^{-1})^T \nabla L(x_k + u a_k d_k, \lambda_*) - \bar{w}_k \\ &= Z_k^{-1} \bar{w}_k Z_k s_k + O(\|s_k\| + \alpha_k \|p_Y\|) + \alpha_k Z_k^{-1} \bar{w}_k Y_k p_Y - \bar{w}_k, \end{aligned} \quad (2.11)$$

where we have defined

$$Z_k^T \tilde{W}_k = \int_{J_0}^1 V_{xx}^2 L(x_k + T a_k d_k, X.) dr. \quad (2.12)$$

Thus

$$s^T y_k = s^T_k \{ Z_k^T \tilde{W}_k Z_k \} s_k + O(a_k) \|s_k\| + [a_k s^T_j (Z_j W_k \tilde{Y}_k) p_Y - \#57^*] + O(o_k) \|a_k\| \|p_Y\|. \quad (2-13)$$

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

Update Criterion I.

Choose a constant $\gamma_{fd} > 0$ and a sequence of positive numbers $\{j_k\}$ such that $E_j \wedge^{\wedge} f_c < \infty$ (this is the same sequence $\{7^*\}$ that was used in (2.10)).

- If W_k is computed by Broyden's method, and if both $s^T y_k > 0$ and

$$\|b_{vll}\| \leq 7^{*2} IM \quad (2.14)$$

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

- // W_k is computed by finite differences, and if both $s^T y_k > 0$ and

$$\|p_Y\| \leq \gamma_{fd} \|p_Z\| / \sigma_1^{1/2} \quad (2.15)$$

hold at iteration k , then update the matrix B_k by means of the BFGS formula (1.22) with S_k and y_k given by (1.20). Otherwise, set $B_{k+i} = B_k$.

Here O_k 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 $(\|Z_j\|_{Titell} + \|cfc\|)$. Moreover, define

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

Prom Byrd and Nocedal (1989), the behavior of $\cos \theta_k$ 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 $k > 1$, $S_k \wedge^0$ and

$$\frac{T}{\sigma_k} \wedge^{\wedge} s_k \geq m > 0 \quad (2.17)$$

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

Then, there exist constants $\beta_2, \beta_3 > 0$ such that, for any $k \geq 1$, the relations

$$\cos \theta_j \geq \beta_2 \tag{2.19}$$

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

hold for at least $\lfloor n/2 \rfloor$ values of $j \in [1, n]$.

This theorem refers to the iterates for which BFGS updating takes place, but since for the other iterates $B_{k+1} = \mathcal{E}^*$, the theorem characterizes the whole sequence of matrices $\{B_k\}$. Theorem 2.1 states that, if $s^T y^*$ 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 $\cos \theta_j$ is bounded away from zero and $B_j s_j = O(\|s_j\|)$. 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", and define $J_k = \{j \in [1, n] : j \in J\}$.

Note that if the matrices B_k are updated only a finite number of times, their condition number is bounded, and (2.19)-(2.20) are satisfied for all k . 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 $Z^T W Z$ is positive definite, then for all x_k in a neighborhood of x^* the smallest eigenvalue of $Z^T W Z$ is bounded away from zero (\bar{W} is defined in (2.12)). We now show that in such a neighborhood with ϵ sufficiently small that Update Criterion I implies (2.17)-(2.18). For the case when \bar{w} is computed by Broyden's method. Using (2.13), (2.14) and (2.10), and since γ^* converges to zero, we have

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

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

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

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

$$\begin{aligned}
 y_k &= Z_{k+1}^T g_{k+1} - Z_k^T g_k - \bar{w}_k \\
 &= Z_{k+1}^T \nabla L(x_{k+1}, \lambda_*) - Z_k^T \nabla \\
 &\quad L(x_k, A) - a_k [Z_{k+1}^T \nabla L(x_k + Y_k p_Y, A) - \nabla L(x_k, A)] \\
 &= (Z_{k+1} - Z_k)^T \nabla L(x_k + Y_k p_Y, A) + Z_k^T (\nabla L(x_k + Y_k p_Y, A) - \nabla L(x_k, A)) \\
 &\quad - a_k [Z_{k+1}^T \nabla L(x_k + Y_k p_Y, A) - Z_k^T \nabla L(x_k + Y_k p_Y, A)] \\
 &\quad + Z_k^T (\nabla L(x_k + Y_k p_Y, A) - \nabla L(x_k, A)) \\
 &= Z_k^T \tilde{W}_k Z_k s_k + a_k Z_k^T (\tilde{W}_k - \hat{W}_k) Y_k p_Y + O(a_k) \|s_k\| \\
 &= Z_k^T \tilde{W}_k Z_k s_k + O(a_k) \|s_k\|.
 \end{aligned}$$

assuming $Y_k p_Y = O(a_k)$. 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, $s^T y_k$ is sufficiently positive, as stipulated by (2.17)-(2.18).

2.4. A Multiplier-free Approach for Choosing n_k .

We will choose α so that for some $p > 0$,

$$\|M^*(x_k)\| \geq \|A^*(x_k)M^*(x_k)\| + p \|c^*(x_k)\| \quad (2.23)$$

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 λ merit function in the direction d^* is given by

$$D^{\lambda}(x_k; d_k) = g^T d_k - W^T d_k. \quad (2.24)$$

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

$$g(x)^T Y(x) p_Y = \lambda(x)^T c(x). \quad (2.25)$$

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

Theorem 2.1 Assume that $A(x)$ is of full column rank for all $x \in D$ and that $Z(x)$ is norm bounded. If $(p^{\lambda}(x))$ is defined by (1.7) and $f(x)$ satisfies (2.23) for all $x \in D$, then $D^{\lambda}(x; d) > 0$ for all d satisfying $\tilde{c}(x) + A(x)^T d = 0$ if and only if x is a Kuhn-Tucker point.

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

$$\begin{aligned} 0 \leq D\phi_\mu(\bar{x}; d) &= \bar{g}(x) f d - n \|c(\bar{x})\|_1 \\ &= \bar{g}(\bar{x})^T Z(\bar{x}) p_z - \beta \|c(\bar{x})\|_1 + X \bar{f}(\bar{x})^T c(\bar{x}) \\ &\leq \bar{g}(\bar{x})^T Z(\bar{x}) p_z - \beta \|c(\bar{x})\|_1 \\ &\leq g(\bar{x})^T Z(\bar{x}) p_z \end{aligned} \quad (2.26)$$

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

$$\begin{aligned} 0 \leq Z^0(\bar{x}; d) &= \bar{f}(\bar{x})^T c(\bar{x}) - \beta \|c(\bar{x})\|_1 \\ &\leq -\beta \|c(\bar{x})\|_1 \\ &< 0. \end{aligned} \quad (2.27)$$

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

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

into the directional derivative:

$$\begin{aligned} D^{\wedge}(x; \langle f \rangle) &= -g(x)^T Z(x) p_z - \beta \|c(x)\|_1 + H(x)^T c(x) \\ &= 0. \end{aligned} \quad (2.29)$$

D

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

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

Now from (1.23) we have that

$$B_k S_k = -O L_k (Z_k^T g_k + \zeta_k w_k) \quad (2.31)$$

As shown in our previous paper,

$$\cos \theta_k = \frac{-(Z_k^T g_k + \zeta_k w_k)^T p_z}{\|2 \zeta_k w_k + \lambda_k\| \|p_z\|} \quad (2.32)$$

If we satisfy the following property for f_k :

$$H_k \|c_k\| \geq \beta \|c_k\| + 2\beta \|c_k\| \quad (2.33)$$

or, equivalently, from (2.25):

$$\|w_k\| \geq \frac{1}{\beta_3} \|g_k + \zeta_k w_k\| + 2\rho \|c_k\| \quad (2.34)$$

then substituting in (2.30), leads to:

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

Note also from (2.31) that

$$\frac{\|g_k\|}{\|B_k g_k\|} = \frac{\|g_k\|}{\|Z_k^T g_k + \zeta_k w_k\|}. \quad (2.36)$$

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

$$\frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\| \leq \|p_z^{(j)}\|, \quad \frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\| \leq \|p_z^{(j)}\| \quad (2.37)$$

Using this and (2.19) in (2.35) we obtain, for $j \in J$,

$$\begin{aligned} D\phi_{\mu_j}(x_j; d_j) &\leq -\frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\|^2 \cos \theta_j - \zeta_j w_j^T p_z^{(j)} - 2\rho \|c_j\|_1 \\ &\leq -\frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\|^2 \cos \theta_j - \zeta_j w_j^T p_z^{(j)} - 2\rho \|c_j\|_1, \end{aligned}$$

where we have dropped the non-positive term $-\zeta_j w_j^T p_z^{(j)}$. Since we can assume that $\beta_3 > 1$ (it is defined as an upper bound in (2.20)), we have

$$D\phi_{\mu_j}(x_j; d_j) \leq -\frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\|^2 \cos \theta_j - 2\rho \|c_j\|_1$$

It is now clear that if

$$2C_j \cos \theta_j \|g_j + \zeta_j w_j\| - C_j w_j^T p_z^{(j)} \leq 2\rho \|c_j\|_1, \quad (2.38)$$

then for all $j \in J$,

$$D\phi_H(x_j; d_j) \leq -\frac{1}{\beta_3} \|Z_j^T g_j + \zeta_j w_j\|^2 - 2\rho \|c_j\|_1. \quad (2.39)$$

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

We will choose β_3 so that (2.38) holds for all iterations. To see how to do this we note from (1.23) that

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

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

$$Ck[2\cos\theta_k |g_k^T Z_k w_k| + w_k^T B^T Z_k g_k + Ck w_k^T B^T w_k] \leq \rho \|c_k\|_1. \quad (2.40)$$

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

$$\epsilon_k = \min\{1, C\hat{c}_k\} \quad (2.41)$$

where \hat{c}_k is the largest value that satisfies (2.40) as an equality.

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

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

Note that for $c_k = 0$, $\hat{c}_k = 1$ and thus μ_k is only updated when $c_k \neq 0$.

The damping factor ϵ_k^* and the updating formula for the penalty parameter μ_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 ϵ_k^* we have in particular

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

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

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

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 $\epsilon \in (0, 1/2)$, $p > 0$ and r, r' 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 $\{\tau_k\}$. Set $k := 1$ and choose a starting point x_i , an initial value $\lambda > 0$ for the penalty parameter, an $(n - m) \times (n - m)$ symmetric and positive definite starting matrix B and an $(n - m) \times n$ starting matrix S .

2. Evaluate λ_k, τ_k, c^* and A_k , and compute p_Y and Z^* .

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

$$(A_k Y_k) p_Y = -c^*. \quad (\text{range space step}) \quad (2.44)$$

4. Calculate u_k^* 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

$$B_k p_z = -\tau_k \bar{g}_k + C_k W_k \quad (\text{null space step}) \quad (2.45)$$

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

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

8. Define the search direction by

$$d_k = Y_k p_Y + Z_k p_z \quad (2.46)$$

and set $\alpha = 1$.

9. Test the line search condition

$$\langle \nabla f(x_k + \alpha d_k) | d_k \rangle \leq \langle \nabla f(x_k) | d_k \rangle + \alpha \lambda C_k \|\nabla f(x_k)\|. \quad (2.47)$$

10. If (2.47) is not satisfied, choose a new $\alpha \in [r \alpha, r' \alpha]$ and go to 9; otherwise set

$$x_{k+1} = x_k + \alpha d_k \quad (2.48)$$

11. Evaluate $\lambda_{k+1}, \tau_{k+1}, c_{k+1}^*$, A_{k+1} , and compute Y_{k+1} and Z_{k+1} .

12. Update λ_k so as to satisfy (2.42).

13. Update λ_{k+1} using equations (2.5) to (2.7). If $findiff = false$ calculate u_{k+1}^* by Broyden's method through equations (2.8) and (2.10); otherwise calculate W_{k+1} by (2.2).

14. If $s^0 y_k \leq 0$ or if (2.15) is not satisfied, set $B^{k+1} = B_k$. Else, compute

$$s^* = -Pz, \quad (2.49)$$

$$V_k = Zl_{ig}(x_k+i) - Zlg(x_k) - \bar{w}_k, \quad (2.50)$$

and compute B_{k+1} by the BFGS formula (1.22).

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

3. Convergence Results

In this section we summarize several convergence results for Algorithm I. Many of the results of 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 $\langle f \rangle^*$ 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 $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $c : \mathbb{R}^n \rightarrow \mathbb{R}^m$ and their first and second derivatives are uniformly bounded in norm over D .
- (II) The matrix $A(x)$ has full column rank for all $x \in D$, and there exist constants γ_0 and γ_1 such that

$$\|A(x)\| \geq \gamma_0, \quad \|Z(s)\| \leq \gamma_1, \quad (3.1)$$

for all $x \in D$.

- (III) For all $k \geq 1$ for which B_k is updated, (2.17) and (2.18) hold.
- (IV) The correction term t^* is chosen so that there is a constant $K > 0$ such that for all

$$\|w_k\| \leq K \|t^*\|^2. \quad (3.2)$$

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 $\|g_j\| = \gamma_j$, is constant for all sufficiently large j , then there is a positive constant γ such that for all large $j \in J$,

$$\phi_\mu(x_j) - \phi_\mu(x_{j+1}) \geq \gamma M [\|g_j\|^2 + \|c_j\|]. \quad (3.3)$$

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 $\{\alpha_k\}$ are constant for all sufficiently large k and $\lim_{k \rightarrow \infty} (\|Z_k^T g_k\| + \|c_k\|) = 0$.

Proof. First note that by Assumptions 3.1 (I)-(II) and (2.25) that $\{\|Z_k^T p_k\| / \|c_k\|\} = \{\|g_k\| / \|c_k\|\} \wedge \{1/\alpha_k\}$ is bounded. Therefore, since the procedure (2.42) increases α_k by at least p whenever it changes the penalty parameter, it follows that there is an index k_0 and a value γ such that for all $k > k_0$, $\|Z_k^T g_k\| \geq \gamma \|c_k\|$. 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 $\langle f \rangle_n(x_k)$ decreases at each iterate, we have that for $k \in J$,

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

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

$$\lim_{j \in J} (\|Z_j^T g_j\| + \|c_j\|) = 0. \quad (3.4)$$

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

$$\lim (\|Z_k^T g_k\| + \|c_k\|) = 0.$$

□

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 α^* is chosen large enough, then x^*

is a point of attraction for the sequence of iterates $\{x_k\}$ 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.

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

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

(1) The functions $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and $c : \mathbb{R}^n \rightarrow \mathbb{R}^m$ are 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 $A^* \in \mathbb{R}^m$ such that

$$V_L(z^*, A^*) = g(x_m) + A^* \lambda^* = 0.$$

(3) For all $q \in \mathbb{R}^{n-m}$, $q^T G^* q > 0$.

(4) There exist constants γ_0, γ_c and γ_G such that, for all x in a neighborhood of x^* ,

$$\|Y(x)Z(x)\| \leq \gamma_0, \quad \|Z(x)\| \leq \gamma_c, \quad (3.6)$$

and

$$\|Y(x)Z(x)\| \leq \gamma_c. \quad (3.7)$$

(5) $Z(x)$ and $Y(x)$ are Lipschitz continuous in a neighborhood of x^* , i.e. there exist constants γ_z and γ^* such that

$$\|\lambda(x) - \lambda(z)\| \leq \gamma_\lambda \|x - z\|, \quad (3.8)$$

$$\|Z(x) - Z(z)\| \leq \gamma_z \|x - z\|, \quad (3.9)$$

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 $q \in \mathbb{R}^{n-m}$,

$$m\|q\|^2 \leq q^T G(x) q \leq M\|q\|^2, \quad (3.10)$$

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^*

$$\|Z(x)^T g(x)\| \leq \|c(x)\| + \gamma_2 \|x - x^*\|, \quad (3.11)$$

for some positive constants γ_1, γ_2 .

This result states that, near x^* , 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 $\gamma_3 > 0$ and $\gamma_4 > 0$, such that for all x sufficiently near x^*

$$\|Z(x)^T g(x)\|^2 \leq M^x \sim M^{x^*} \leq \gamma_4 (\|Z(x)^T g(x)\|^2 + \|c(x)\|). \quad (3.12)$$

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

$$\|Z(x)^T g(x)\| = \|Z(x)^T [f(x) + \lambda c(x)]\| \quad (3.13)$$

$$= \|Z(x)^T f(x) + \lambda Z(x)^T c(x)\| \quad (3.14)$$

$$\geq L(x, \lambda) + \lambda \|c(x)\| \quad (3.15)$$

$$\geq L(x, \lambda) + \lambda \|c(x)\| \quad (3.16)$$

$$(3.17)$$

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

$$\begin{aligned} \phi_\mu(x) - \phi_\mu(x^*) &\geq \nabla L(x^*, \lambda^*)^T (x - x^*) + \frac{1}{2} (x - x^*)^T \nabla_{xx}^2 L(x^*, \lambda^*) (x - x^*) \\ &\quad + \lambda \|c(x)\| + \frac{1}{2} \|c(x)\|^2 - \frac{1}{2} \|c(x^*)\|^2 + O(\|x - x^*\|^3) \end{aligned} \quad (3.18)$$

Now we note that

$$\lambda \|c(x)\| = \frac{1}{2} (x - x^*)^T A_j g(x - x^*) + O(\|x - x^*\|^3). \quad (3.19)$$

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 ν such that:

$$\|(x - x^*)^T (\nabla_{xx}^2 L(x^*, \lambda^*) + \nu A_j A_j^*) (x - x^*)\| \geq 2\gamma_3 \|a_j - x^* f\| \quad (3.20)$$

Now since there exists a $K_c > 0$ such that $\|c(a_j)\| \leq K_c \|x - x_m\|$ we have for $\|x - x^*\| \leq p/(2\nu K_c)$:

$$\phi_\mu(x) - \phi_\mu(x^*) \geq 2\gamma_3 \|x - x^*\|^2 + \frac{1}{2} \|c(x)\| + O(\|x - x^*\|^3) \quad (3.21)$$

$$\geq \frac{1}{2} \|c(x)\| \quad (3.22)$$

$$(3.23)$$

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

$$M(x) - \frac{1}{2} \|c(x)\|_1^2 = \frac{1}{2} \|c(x)\|_1^2 + H\|c(x)\|_1^2 - \frac{1}{2} \|c(x)\|_1^2 \quad (3.24)$$

$$= L(x, A) - f(x) + M\|c(x)\|_1^2 - H\|c(x)\|_1^2 \quad (3.25)$$

$$\leq O(\|x - x^*\|^2) + p\|c(x)\|_1 \quad (3.26)$$

$$\leq \gamma_4 [\|Z(x)^T \nabla g(x)\|^2 + \|c(x)\|_1] \quad (3.27)$$

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 , $\langle \nabla M(x), x - x^* \rangle \leq 0$ for all $x \in [0, 1]$. In other words, $x - x^*$ is in the connected component of the level set $\{x : \langle \nabla M(x), x - x^* \rangle \leq 0\}$ 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 x_{k_0} is sufficiently close to a solution point x^* that satisfies Assumptions 3.2, and if the weight β_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 $\|A^{-1}\|$ is bounded. Therefore the procedure (2.42) ensures that the weights β_k are constant, say $\beta_k = \beta_0$ for all large k . 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 β_0 , 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 $\epsilon > 0$, there is an iterate x_{k_0} such that

$$\|x_{k_0} - x^*\| \leq \frac{\gamma_3}{\gamma_2 \gamma_4 \beta_0} \epsilon^2,$$

where β_0 is such that $\| \cdot \|_1 \leq \beta_0 \| \cdot \|_2$. Assumption 3.3 shows that for any $k \geq k_0$, x_k is in the connected component of the level set of x_{k_0} that contains x_{k_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) $\|x_k - x_*$ $\leq \gamma_3^{-\frac{1}{2}} (\phi_\mu(x_k) - \phi_\mu(x_*))^{1/2}$ for $k \geq k_0$, and since we can assume that $\|Z_{k_0}^T g_{k_0}\| \leq 1$ we have from Lemmas 3.3 and 3.4, for any $k \geq k_0$

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

This implies that the whole sequence of iterates remains in a neighborhood of radius ϵ of x_* . If ϵ is small enough we conclude by (3.12), by the monotonicity of $\{\phi_\mu(x_k)\}$ and Theorem 4.2 that the iterates converge to x_* .

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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 $p > 0$, $\|x_k - x_*\| \leq p \|x_{k-1} - x_*\|$ and

$$\|c(x_k)\| \geq \|c(x_{k-1})\| + p M \|x_{k-1} - x_*\| \quad (3.28)$$

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,

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

and let

$$U_k = \{j \in U : j \geq k\}. \quad (3.30)$$

The number of elements in U_k will be denoted by $|U_k|$. 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 $k \in U$ and any $j \geq k$*

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

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

This result implies that if $\{U_k/k\}$ is bounded away from zero, then Algorithm I is R-linearly 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 $\{U_k/k\} \rightarrow 0$. We therefore need to examine the iteration more closely.

We make use of the matrix function ψ defined by

$$\psi(B) = \text{tr}(B) - \ln(\det(B)), \quad (3.32)$$

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

$$\text{Incond}(B) < V > (\epsilon), \quad (3.33)$$

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

$$Vk = G^{1/2} y_k, \quad \tilde{s}_k = G^T J^2 s_k, \quad (3.34)$$

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

$$\cos \tilde{\theta}_k = \frac{\tilde{s}_k^T \tilde{B}_k \tilde{s}_k}{\|\tilde{s}_k\| \|\tilde{B}_k \tilde{s}_k\|}, \quad (3.36)$$

and

$$\tilde{q}_k = 2 \frac{G}{s_k} \wedge s_k. \quad (3.37)$$

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

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

This expression characterizes the behavior of the BFGS matrices B_{k_j} 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 are used to estimate w_k and TU^A , these are accurate to second order.

Lemma 3.7 // at the iterate x_k , the corrections w_k and \tilde{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

$$\|\tilde{w}_k\| = O(\|b_k\|), \quad (3.39)$$

$$\|K - Z;^T W; y_{fc} p_Y\| = O(\alpha_k \|p_Y\|). \quad (3.40)$$

and

$$\|\tilde{w}_k - \alpha_k Z^T W; Y_k p_Y\| = O(\sigma_k \|p_Y\|). \quad (3.41)$$

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

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

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

$$VL(x_k + Y_k p_Y, A) = O(\|x - x_m\|) + O(\|b_Y\|) = O(a_k) \tag{3.43}$$

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

$$[Z_k^T \bar{W}_k - Z_k^T W_k] Y_k p_Y = O(\|b_Y\|) \|p_Y\| \tag{3.44}$$

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 $\{\|B^k\|\}$ and $\{\|B^k\|^{-1}\}$ are bounded, and for all $k \in U$*

$$\|(B_k - Z_k^T \bar{W}_k) p_Z\| = o(\|d_k\|). \tag{3.45}$$

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 B_k takes place. We have from (2.50), (2.48), (2.46), (2.12) and (2.49)

$$\begin{aligned}
y_k &= Z_{k+1}^T g_{k+1} - Z_k^T g_k - \bar{w}_k \\
&= Z_{k+1}^T \nabla L(x_{k+1}, X) - Z_k^T [VL(x_k, X) - \bar{w}_k] \\
&= (Z_{k+1} - Z_k)^T VL(x_{k+1}, A) + Z_{k+1}^T VL(x_{k+1}, A) - VL(x_k, A) - \bar{w}_k \\
&= (Z_{k+1} - Z_k)^T VL(x_{k+1}, A) + [Z_{k+1}^T \int_0^1 V_{xx}^2 L(x_k + T a_k d_k, A) r dr] a_k d_k - \bar{w}_k \\
&= c_{T_k} Z_k^T \bar{W}_k (Z_k p_Z + Y_k p_Y) - \bar{w}_k + O(\tau_{fc} (\|a_k\| + a_k \|p_Y\|)) \\
&= Z_k^T \bar{W}_k Z_k p_Z + a_k [Z_k^T \bar{W}_k - Z_k^T W_k] Y_k p_Y + (a_k Z_k^T W_k Y_k p_Y - \bar{w}_k) \\
&\quad + O(a_k (\|s_k\| + a_k \|p_Y\|)).
\end{aligned} \tag{3.46}$$

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 $\|Z\|\bar{W}_k - Z_j W_{fc}\| = O(o_k)$, and from (2.10) we have that $\bar{w}_k = O(\|p_Y\|/7fc)$. Using this and Assumptions 3.2 in (3.46) we have

$$\begin{aligned} y_k &= Z\bar{W}_k Z_k s_k + \{a_k + l + 1/7^*\}O(a^*\|p_Y\|) + O(a_k)\|s_k\| \\ &= (Z\bar{W}_k Z_k - G_*)s_k + G_* s_k + (a^* + 1 + 1/\gamma_k)O(\alpha_k\|p_Y\|) + O(\sigma_k)\|s_k\| \end{aligned} \quad (3.47)$$

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

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

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

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

Similarly from (3.47) and (3.34) we have

$$\begin{aligned} \tilde{y}_k^T \tilde{y}_k &\leq \|(Z_k^T \bar{W}_k Z_k - G_*)s_k\|^2 \|G_*^{-1}\| \\ &\quad + 2(1 + O(a_k))\|(Z\bar{W}_k Z_k - G_*)s_k\| \|G_*^{1/2}\| \|s_k\| + (l + O(a_{fc}))^2 \|s_k\|^2 \\ &\quad + 2(\sigma_k + 1 + 1/\gamma_k)O(\|\alpha_k p_Y\|)\|G_*\| (\|s_k\| + \|2\bar{W}_k Z_k - G_*\| \|s_k\| \|G_*^{-1/2}\|) \\ &\quad + (\sigma_k + 1 + 1/\gamma_k)^2 O(\|\alpha_k p_Y\|)^2, \end{aligned} \quad (3.49)$$

and thus

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

At this point we invoke the update criterion, and note from (2.14) that if BFGS updating of B_k takes place at iteration fc , then $\|afcp_Y\| \leq 7fc\|sfc\|$ where $\{7^*\}$ is summable. Using this, the assumption that o_k converges to zero, and (3.48) we see that for large k

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

and using (3.50)

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

Therefore

$$\frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} = \frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} = 1 + O(\sigma_k + \gamma_k). \quad (3.52)$$

We now consider $x > \tilde{B}_k + i$ given by (3.38). A simple expansion shows that for large \tilde{B}_k , $\ln(1 + O(a_k + 7_{fc})) = O(a_k + 7_{fc})$. Using this, (3.51) and (3.52) we have

$$4 > \tilde{B}_M = 1 > \tilde{B}_k + O(a_k + 7_{fc}) + \ln \cos^2 \tilde{\theta}_k + \left[1 - \frac{1}{\cos^2 \tilde{\theta}_k} \ln \frac{1}{\cos^2 \tilde{\theta}_k} \right]. \quad (3.53)$$

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

$$iK\tilde{B}_M < a_k + 7_{fc}. \quad (3.54)$$

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 \tilde{w}_k is computed by finite differences. In this case (2.15) holds. Again we begin by considering (3.46),

$$y_k = Z_k^{-1} \tilde{W}_k^{-1} (Z_k^{-1} \tilde{W}_k^{-1} Y_k p_Y + (\alpha_k Z_k^{-1} \tilde{W}_k^{-1} Y_k p_Y - \tilde{w}_k)) + O(\sigma_k)(\|s_k\| + \alpha_k \|p_Y\|).$$

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

$$\begin{aligned} y_k &= Z_k^{-1} \tilde{W}_k^{-1} Z_k s_k + O(\sigma_k)(\|s_k\| + \alpha_k \|p_Y\|) \\ &= \{Z_k^{-1} \tilde{W}_k^{-1} Z_k - G_k\} s_k + G_k s_k + O(a_k)(\|s_k\| + a_k \|p_Y\|). \end{aligned} \quad (3.55)$$

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

$$\tilde{y}_k \tilde{s}_k = s_k \{Z_k^{-1} \tilde{W}_k^{-1} Z_k - G_k\} s_k + \|h\|^2 + O(a_k)(\|\tilde{s}_k\|^2 + \alpha_k \|p_Y\| \|\tilde{s}_k\|),$$

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

$$\begin{aligned} \frac{\tilde{y}_k \tilde{s}_k}{\|\tilde{s}_k\|^2} &= 1 + \frac{s_k^T \{Z_k^{-1} \tilde{W}_k^{-1} Z_k - G_k\} s_k}{\|s_k\|^2} + O(a_k) \left(1 + \frac{\alpha_k \|p_Y\|}{\|i_k\|} \right) \\ &= 1 + O(\sigma_k) + O\left(\sigma_k \frac{\alpha_k \|p_Y\|}{\|\tilde{s}_k\|}\right). \end{aligned} \quad (3.56)$$

Similarly from (3.55) and (3.34) we have

$$\begin{aligned} \tilde{y}_k^T \tilde{y}_k &< \|\tilde{Z}_k^T \tilde{W}_k \tilde{Z}_k - G_k\|_{S_k} \|\tilde{G}_k\| \\ &+ 2(1 + O(a_k)) \|\tilde{Z}_k^T \tilde{W}_k \tilde{Z}_k - G_k\|_{S_k} \|\tilde{G}_k\|^{1/2} \|\mathbf{p}^*\| + (1 + O(a_k)) \|\tilde{s}_k\|^2 \\ &+ \sigma_k O\left(\|\alpha_k \mathbf{p}_Y\| \|\tilde{G}_k\|^{-1/2} \left[\|(1 + O(a_k)) \|\tilde{s}_k\| + \|(Z_k^T \tilde{W}_k Z_k - G_k)_{S_k}\| \|\tilde{G}_k\|^{-1/2}\|\right]\right) \\ &+ 4O(\|a_{kPY}\|)^2, \end{aligned}$$

and thus

$$\frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} < 1 + O(a_k) + \frac{a_k O(\|\mathbf{p}_Y\|)}{\|\tilde{s}_k\|} + o\left(\frac{\|\alpha_k \mathbf{p}_Y\|^2}{\|\tilde{s}_k\|^2}\right). \quad (3.57)$$

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 $\|\mathbf{p}_Y\| \leq 7fd\|Pz\|/cric^2$. 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

$$\|\tilde{y}_k\|^2 \|\tilde{s}_k\|^2 \sim n(n-1)^2 \quad \text{rtW}$$

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

$$\psi(\tilde{B}_{k+1}) = \psi(\tilde{B}_k) + O(a_k^{1/2}) + \ln \cos^2 \theta_k + \ln \frac{1 - \cos^2 \theta_k}{\cos^2 \theta_k} + \ln \frac{1 - \cos^2 \theta_k}{\cos^2 \theta_k}. \quad (3.59)$$

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

$$\psi(\tilde{B}_{k+1}) < \psi(\tilde{B}_k) + O(a_k^{1/2}). \quad (3.60)$$

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^I corresponds to the iterates in which \tilde{w}_k is computed by Broyden's method, and U^II to the iterates in which finite differences are used. We also define $U^I_k = U^I \cap \{1, 2, \dots, A\}$ and $U^II_k = U^II \cap \{1, 2, \dots, fc\}$.

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

$$\psi(\tilde{B}_{k+1}) \leq \psi(\tilde{B}_1) + C_1 \sum_{j \in U^I_k} a_j^{1/2} + C_2 \sum_{j \in U^II_k} Y_j + C_3 \sum_{j \in U^II_k} \mathbf{1}. \quad (3.61)$$

for some constants C_1, C_2, C_3 . By (3.31) and since $|U_j'| \leq |U_j|$,

$$\begin{aligned} \mathbf{E}^a)^{1/2} \wedge \mathbf{E} \sum_{j \in U''} C^{1/2} \tau^{1/2} |U_j|^{1/2} \\ \leq \sum_{j \in U''} C^{1/2} \tau^{1/2} |U_j'|^{1/2} \\ = \sum_{i=1}^{|U''|} C^{1/2} \tau^{1/2} \\ < \infty. \end{aligned}$$

Similarly

$$\mathbf{E} \sum_{j \in U'} i < \infty,$$

and since $\{7^*\}$ is summable we conclude from (3.61) that $\{xp(\bar{B}_k)\}$ is bounded above. By (3.32) $\langle \bar{B}_k \rangle = \text{SJLiCt}'' - \ln \langle \bar{B}_k \rangle$ where Z_j are the eigenvalues of i^* , and it is easy to see that this implies that both $\text{H}^* \Pi$ and $\text{H} \bar{B}^{\wedge 1}$ are bounded.

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

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

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

$$\lim_{k \rightarrow \infty} \ln \cos^2 \bar{\theta}_k = 0,$$

and

$$\lim_{k \rightarrow \infty} \left[1 - \frac{\bar{q}_k}{\cos^2 \bar{\theta}_k} + \ln \frac{\bar{q}_k}{\cos^2 \bar{\theta}_k} \right] \rightarrow 0.$$

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

$$\lim_{k \rightarrow \infty} \cos^2 \bar{e}_k = \lim_{k \rightarrow \infty} \bar{g}_k = 1. \quad (3.62)$$

Now from (3.36)-(3.37)

$$\begin{aligned} \frac{\|G^{\wedge 1/2} (B_k - G) p_z\|^2}{\|G^{\wedge 1/2} p_z\|^2} &= \frac{\|(B_k - I) \bar{s}_k\|^2}{\|\bar{s}_k\|^2} \\ &= \frac{\|B_k \bar{s}_k\|^2 - 2i \wedge B_k \bar{s}_k + \bar{s}_k^T \bar{s}_k}{\bar{s}_k^T \bar{s}_k} \\ &= \frac{\bar{q}_k^2}{\cos^2 \bar{\theta}_k} - 2\bar{q}_k + 1. \end{aligned}$$

It is clear from (3.62) that the last term converges to 0 for $k \rightarrow \infty$, 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 $\{x^k\}$ 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 $\{B^k\}$ 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^k 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 \bar{x}^k , and using appropriate update criteria, Algorithm I is 2-step Q-superlinearly convergent. This was proved by Nocedal and Overton (1985) assuming that Y^k and Z^k are orthogonal bases, and that a good starting matrix B_0 is used. This result has been extended by Xie (1991) for more general bases and for any positive definite starting matrix B_0 .

To establish 1-step superlinear convergence we need to assume that the steplengths α_k have the value 1 for all large k . 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 ℓ_1 merit function (1.7) used in this paper may reject steplengths of one, even though the lower bound on α_k is weaker than $\|A\|^{-1}$. 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 k . 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 k , 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 1 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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