Analysis of a Reversed Cdeman-Conn Reduced SOP Method

LT.Biegler

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ANALYSIS OF A REVERSED COLEMAN-CONN REDUCED SQP METHOD

by

Lorenz T. Biegler
Chemical Engineering Department
Carnegie Mellon University
Pittsburgh, PA 15213
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ABSTRACT

We propose a quasi-Newton algorithm for solving large optimization problems with nonlinear equality constraints. It is designed for problems with few degrees of freedom, and is motivated by the need to use sparse matrix factorizations. The algorithm incorporates a correction vector that approximates the cross term Z^TWYp_Y in order to estimate the curvature in both the range and null spaces of the constraints. The algorithm can be considered to be, in some sense, a practical implementation of an algorithm of Coleman and Conn. We give conditions under which local and superlinear convergence is obtained.

Key words: successive quadratic programming, reduced Hessian methods, constrained optimization, quasi-Newton method, large-scale optimization.

Abbreviated title: A Reversed Coleman-Conn Method

1. Introduction.

We consider the nonlinear optimization problem

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

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

where $f : \mathbf{R}^n \to \mathbf{R}$ and $c : \mathbf{R}^n \to \mathbf{R}^m$ are smooth functions. We assume that the first derivatives of f and c are available, but our algorithm does not require second derivatives.

The successive quadratic programming (SQP) method for solving (1.1)-(1.2) generates, at an iterate x_k, a search direction d_k by solving

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

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

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

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

A new iterate is then computed as

$$x_{k+1} = x_k + \alpha_k d_k, \tag{1.6}$$

where a_k is a steplength parameter chosen so as to reduce the value of the merit function. In this study we continue to use the £\ merit function

$$<l>_{fl}(x) \wedge f(x) +_f i \backslash\backslash c(x) \backslash\backslash_u \tag{1.7}$$

where $\backslash i$ is a penalty parameter; see for example Conn (1973), Han (1977) or Fletcher (1987). We could have used other merit functions, but the essential points we want to convey in this article are not dependent upon the particular choice of the merit function.

The solution of the quadratic program (L3)-(1.4) can be written in a simple form if we choose a suitable basis of R^n to represent the search direction d_k. For this purpose, we introduce a nonsingular matrix of dimension n, which we write as

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

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

$$A \backslash Z_k = 0. \tag{1.9}$$

(From now on we abbreviate $A(x_k)$ as A_{ky} $g(x_k)$ 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

$$d_k = Y_k p_Y + Z_k p_Z, \tag{1.10}$$

for some vectors p_Y 6 R^m and p_z e $R^{n \sim m}$. Due to (1.9) the linear constraints (1.4) become

$$c_k + Al\, Y_k p_Y = 0. \tag{1.11}$$

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 $A_k^T Y_k$ is nonsingular, so that p_Y is determined by (1.11):

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

Substituting this in (1.10) we have

$$d_k = -Y_k [Al Y_k]^{-1} c_k + Z_k p_z. \tag{1.13}$$

Note that

$$Y_k [Al Y_k Y^l \tag{1.14}$$

is a right inverse of $A£$, and that the first term in (1.13) represents a particular solution of the linear equations (1.4).

We have thus reduced the size of the SQP sub-problem which can now be expressed exclusively in terms of the variables p_z. Indeed, substituting (1.10) into (1.3), considering *YkPy* as constant, and ignoring constant terms, we obtain the unconstrained quadratic problem

$$\min_{p_Z \in \mathbf{R}^{n-}} \quad (Z?g_k + ZZW_kY_kp_Y)^T p_z + y_z^T(ZZW_kZ_k)p_z. \qquad (1.15)$$

Assuming that $Z\%W_kZ_k$ is positive definite, the solution of (1.15) is

$$p_z = -(Z_k^T W_k Z_k)^{-l}[ti[g_k + ZlW_kY_kp_Y). \qquad (1.16)$$

This determines the search direction of the SQP method.

We are particularly interested in the class of problems in which the number of variables n is large, but n - m is small. In this case it is practical to approximate $Z][\backslash V_kZ_k$ using a variable metric formula such as BFGS. On the other hand, the matrix $Z\%W_kY_k$, of dimension (n — m) x m may be too expensive to compute directly when m is large. For this reason several authors simply ignore the "cross term" $Zj\backslash V_kY_kp_Y$ in (1.16) and compute only an approximation to the reduced Hessian $Z_k\wedge W_kZ_k\backslash$ see Coleman and Conn (1984), Nocedal and Overton (1985), and Xie (1991). This approach is quite adequate when the basis matrices Y_k and Z_k in (1.8) are chosen to be orthonormal (Gurwitz and Overton (1989)).

Therefore in this paper we approximate the cross term $[Z\wedge W_kY_k]p_Y$ by a vector w_k,

$$\backslash u_k^{T} Vv_kY_k\backslash p_Y \; £3 \; w_k, \qquad (1.17J$$

without computing the matrix $Z][W_kY_k$. Instead we consider a finite difference approximation given by either:

$$w_k = Zl[VL(x_k + Y_kp_Y, X_k) - \mathrm{VL}(a^*, A^*)]. \qquad (1.18)$$

or

$$w_k = Z\{x_k + Y_kp_Y)^T g(x_k + Y_kp_Y) - Zlg_k \qquad (1.19)$$

2. Development of the revised algorithm

We will see that addition of the 'cross term[5] approximation can be done without substantially increasing the cost of the iteration, and we will show that the rate of convergence of the new algorithm is 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 (1.16) of our algorithm will be given by

$$p_z = -\{ZlW_kZ_k)^{\sim l}[Zlg_k + \mathrm{Obtifc}], \qquad (2.1)$$

where $0 < Ok \leq 1$ is a damping factor to be discussed later on.

To approximate the reduced Hessian matrix $Z\wedge W_kZ_k$, $W_k+i = Vl_xL(x_k+i, A^*+i)$, we have that

$$Z_j\, W_{k+1}(x_{k+1} - x_k) \approx Z_k^T[\nabla_x L(x_{k+1}, \lambda_{k+1}) - V_xL\{x_k, A_{fc+1})]_f \qquad (2.2)$$

when *Xk+* is close to x_k- We use this relation to establish the following secant equation for the quasi-Newton approximation to the reduced Hessian *Z^WkZ^*

$$Bk+iSk = yk, \tag{2.3}$$

with *Sk* and y* defined by

$$Sk = OL_kp_z, \tag{2.4}$$

and

$$y_k = zZ\backslash V_xL(x_k+u \text{ Ait-Hi}) - V_xL\{x_k, \text{A*+i})] - \overline{w}_k, \tag{2.5}$$

or

$$Vk = ZZ+_{igk}+i - Zlg_k - \overline{w}_k, \tag{2.6}$$

Here we define

$$\overline{w}_k = \text{a*[ZftVL(x* + npy, A*}_{+1}) - \text{VL(s*,.A*}_{+1})], \tag{2.7}$$

or

$$\overline{w}_k = \text{a}_{fc}[\text{Z(a:ib} + Y_kp_Y)^Tg(x_k + Y_kp_Y) - Z\%g_k], \tag{2.8}$$

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

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}, \tag{2.9}$$

provided $\overline{5\text{^}j\text{/}b}$ is sufficiently positive and use this matrix for the nullspace step:

$$\text{Pz} = -iB_h)^{-1}[2\%g_h + \text{Cfctiifc}], \tag{2.10}$$

We would like to highlight a subtle, but important point. We have defined two correction terms, w_k and $\overline{w}_k$. Both are approximations to the cross term $(Z^TWY)p_y$. The first term, w_{ki} which is needed to define the null space step (2.1) - and thus the new iterate Xjb+i. The second term, $\overline{W}k$, which is used in (2.5) to define the BFGS update of f?*, is computed using the new multiplier A^+i, and also takes into account the steplength a*.

The Lagrange multiplier estimates A* needed in the definition (2.5) of y* will be defined by

$$\lambda_k = -[Y_k^T A_k]^{-1} Y_k^T g_k. \tag{2.11}$$

This formula is motivated by the fact that, at a solution x^* of (1.1)-(1.2), we have - j * = A*A«c, and since Y^jl^Yi]"[1] is a right inverse of *A£*,

$$X. = -\backslash Y?A.]^{-1}Y?g,.$$

Using the same right inverse (1.14) in the definitions of p_Y and A* will allow us a convenient simplification in the formulae presented in the following sections. We stress, however, that other Lagrange multiplier estimates can be used, or multiplier estimates may also be avoided if (1.19), (2.8) and (2.6) are used.

2.1. Update Criterion.

It is well known that the BFGS update (2.9) is well defined only if the curvature condition $s£y_k > 0$ 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 $s_k^T y_k > 0$ can be difficult to obtain, even near the solution.

To see this we first note from (2.5), (2.4) and from the Mean Value Theorem that

$$\begin{aligned} y_k &= Z_k^T \left[\int_0^1 \nabla^2_{xx} L(x_k + \tau\alpha_k d_k, \lambda_{k+1}) d\tau\right] \alpha_k d_k - \bar{w}_k \\ &\equiv Z_k^T \tilde{W}_k \alpha_k d_k - \bar{w}_k \\ &= Z_k^T \tilde{W}_k Z_k s_k + \alpha_k Z_k^T \tilde{W}_k Y_k p_Y - \bar{w}_k \end{aligned} \tag{2.12}$$

where we have defined

$$\tilde{W}_k = \int_0^1 \nabla^2_{xx} L(x_k + \tau\alpha_k d_k, \lambda_{k+1}) d\tau. \tag{2.13}$$

Thus

$$s_k^T y_k = s_k^T \left(Z_k^T \tilde{W}_k Z_k\right) s_k + \alpha_k s_k^T \left[Z_k^T \tilde{W}_k Y_k\right] p_Y - s_k^T \bar{w}_k. \tag{2.14}$$

Near the solution, the first term on the right hand side will be positive since $Z_k^T \tilde{W}_k Z_k$ can be assumed positive definite. Nevertheless the last two terms are of uncertain sign and can make $s_k^T y_k$ negative. Several reduced Hessian methods in the literature set $\bar{w}_k$ equal to zero for all k, and update B_k only if p_Y is small enough compared with s_k that the first term in the right hand side of (2.14) dominates the second term (see Nocedal and Overton (1985), Gurwitz and Overton (1989), and Xie (1991)).

Also, skipping the BFGS update is desirable in some circumstances and we now present a strategy for deciding when to do so. Here we define $\sigma_k = \max\{\|e_k\|, \|e_{k+1}\|\}$ where $e_k = x_k - x_*$ and σ_k converges to zero if the iterates converge to x_*.

Update Criterion I.

Choose a constant $\gamma > 0$ *and a sequence of positive numbers* $\{\gamma_k\}$ *such that* $\sum \gamma_k < \infty$.

- *If* $\bar{w}_k$ *is set to zero and if both* $s_k^T y_k > 0$ *and*
$$\|p_Y\| \le \gamma_k \|p_Z\| \tag{2.15}$$
hold at iteration k, then update the matrix B_k *by means of the BFGS formula (2.9) with* s_k *and* y_k *given by (2.4) and (2.5). Otherwise, set* $B_{k+1} = B_k$.

- *If* $\bar{w}_k$ *is computed by finite differences, and if both* $s_k^T y_k > 0$ *and*
$$\|p_Y\| \le \gamma \|p_Z\| / \sigma_k^{1/2} \tag{2.16}$$
hold at iteration k, then update the matrix B_k *by means of the BFGS formula (2.9) with* s_k *and* y_k *given by (2.4) and (2.5). Otherwise, set* $B_{k+1} = B_k$.

Note that σ_k requires knowledge of the solution vector x_*, and is therefore not computable. However we will later see that σ_k can be replaced by any quantity which is of the same order as the error e_k, for example the optimality conditions $(\|Z_k^T g_k\| + \|c_k\|)$. Nevertheless for convenience we will leave σ_k in (2.16).

We now closely consider the properties of the BFGS matrices B_k when Update Criterion I is used. Let us define

$$\text{cosfr} = / * \overset{T}{?}\text{-}* \; \frac{**}{\backslash\backslash 8k\backslash\backslash \; \backslash\backslash Bk8k\backslash\backslash}, \tag{2.17}$$

which, as we will see, is a measure of the goodness of the null space step *ZkVz-* We begin by restating a theorem from Byrd and Nocedal (1989) regarding the behavior of *cos 6k* when the matrix £* is updated by the BFGS formula.

Theorem 2.1 *Let {Bk} be generated by the BFGS formula (2.9) where, for all k ≥ \ , Sk ^ 0 and*

$$\frac{\%\wedge}{s_k^T s_k} \geq m > 0 \tag{2.18}$$

$$\frac{\|y_k\|^2}{y_k^T s_k} \leq \text{M.} \tag{2.19}$$

Then, there exist constants /3i,02,(h > 0 such that, for any k >1, the relations

$$\text{cos}Oj \quad >\_ \qquad fii \tag{2.20}$$

$$\beta_2 \leq \frac{\|B_j s_j\|}{\|s_j\|} \leq fh \tag{2.21}$$

hold for at least \^k] values of j € [l,fe].

This theorem refers to the iterates for which BFGS updating takes place, but since for the other iterates *Bk+* = B*, the theorem characterizes the whole sequence of matrices {Bit}. Theorem 2.1 states that, if $s\backslash y_k$ is always sufficiently positive, in the sense that conditions (2.18) and (2.19) are satisfied, then at least half of the iterates at which updating takes place are such that *cosOj* is bounded away from zero and *BjSj* = 0(||s;||). 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 (2.20) and (2.21) hold. We call J the set of "good iterates", and define* J_k = Jn {1,2, ...,*&}.

Note that if the matrices B_k are updated only a finite number of times, their condition number is bounded, and (2.20)-(2.21) are satisfied for all *k.* Thus in this case all iterates are good iterates.

We now study the case when BFGS updating takes place an infinite number of times. Assume that all functions under consideration are smooth and bounded. If at a solution point x* the reduced Hessian *ZjW+Z** is positive definite, then for all *x^* in a neighborhood of *x+* the smallest eigenvalue of *Z$_k^\wedge$$\tilde{W}$kZk* is bounded away from zero ($\tilde{W}$* is defined in (2.13)). We now show that in such a neighborhood Update Criterion I implies (2.18)-(2.19).

If *Wk* is computed by the finite difference formula (2.7), we see from (2.5) and the Mean Value theorem that there is a matrix $\hat{W}_k$ such that

$$\begin{aligned} Vk &= 2_k^T[\nabla L(x_{k+1}, \lambda_{k+1}) - \nabla L(x_k + \alpha_k Y_k p_Y, \lambda_{k+1})] \\ &\equiv Z_k^T \hat{W}_k Z_k s_k. \end{aligned}$$

(A slightly more involved relation follows from (2.6).)

Nevertheless, (2.18)-(2.19) 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 *Bk* takes place, sjjTy* is sufficiently positive, as stipulated by (2.18)-(2.19).

2.2. Choosing /J* and Ot-

We will now see that by appropriately choosing the penalty parameter $\backslash i_k$ and the damping parameter 0t for it;*, the search direction generated by our method is always a descent direction for the merit function. Moreover, for the good iterates J, it is a direction of strong descent.

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

$$D4>p_k(x_k;d_k) = gld_k - \text{Ai*ll<*||i.} \qquad (2.22)$$

The fact that the same right inverse of *A£* is used in (1.12) and (2.11) implies that

$$g_k^T Y_k p_Y = \backslash lc_k. \qquad (2.23)$$

Recalling the decomposition (1.10) and using (2.23) we obtain

$$\begin{aligned} D\phi_{\mu_k}(x_k;d_k) &= g_k^T Z_k p_Z - n_k\|c_k\|_1 + \lambda_k^T c_k \\ &= (Z_k^T g_k + \zeta_k w_k)^T p_Z - \zeta_k w_k^T p_Z - \mu_k\|c_k\|_1 + \lambda_k^T c_k. \end{aligned} \qquad (2.24)$$

Now from (2.4) and (2.10) we have that

$$B_k Sk = -ot_k\{Zlg_k + \text{0kW*}). \qquad (2.25)$$

Substituting this in (2.17) we obtain

$$\cos 0, \quad - \frac{-(^TZ k9k+<;_kw_k)^T p_z}{}$$

Recalling the inequality Ajj[c/t ≤ ||Ajb||oo||Qblli. and using (2.26) in (2.24) we obtain, for all *,

$$D<f>\wedge_k(x_k;d_k) \leq -\backslash\backslash ZZg_k + \text{Okay } ||pz||\cos 0^* - Ckwfoz \text{ " (P* ~ l|A*lloo)llQk||i.} \qquad (2.27)$$

Note also from (2.25) and (2.4) that

$$\frac{\|N\|}{\|B_k s_k\|} = \frac{\|p_Z\|}{\|Z_k^T g_k + \zeta_k w_k\|}. \qquad (2.28)$$

We now concentrate on the good iterates *J*, as given in Definition 2.1. If *j* e *J*, we have from (2.28) and (2.21) that

$$\frac{1}{\beta_3}\|Zj_{9j} + CjWjW \leq \|p?\| \leq \frac{1}{\beta_2}\|Z_j^T g_j + C_{jWj}\|. \qquad (2.29)$$

Using this and (2.20) in (2.27) we obtain, for $j \in J$,

$$D\langle t\rangle_N(xy,dj) \leq -\wedge f \quad Z \; g_j + \zeta_j w_j \, f \cos\theta_j - \zeta_k w_j^T p_Z^{(j)} - (\mu_j - \|\lambda_j\|_\infty)\|c_j\|_1$$

$$\leq -\frac{\beta_1}{\beta_3}\|Z_j^T g_j\|^2 - \frac{2\zeta_j \cos\theta_j}{\beta_3}(g_j^T Z_j w_j) - \zeta_j w_j^T p_Z^{(j)} - (\mu_j - \|\lambda_j\|_\infty)\|c_j\|_1,$$

where we have dropped the non-positive term —C^ cos ^jll^{tjL;}ill²//^3- Since we can assume that /?3 > 1 (it is defined as an upper bound in (2.21)), we have

$$Dt\wedge dj) < -\wedge\|ZJ_{gj}\|^2 + \wedge\cos\wedge 1\wedge Z,\wedge! - CjwfpP] - (_H - \text{IIA\^{}UIIqHi.}$$

It is now clear that if

$$2C_j cose_j|gjZ_jw_j| - (jwjpP \leq pWcjWu \qquad (2.30)$$

for some constant p, and if

$$H > Ui\|oo + 2p, \qquad (2.31)$$

then for all $j \in J$,

$$Dt\wedge dj) < -2j\|Zj_{gj}\|^2 - \text{PIIC}\wedge. \qquad (2.32)$$

This means that if (2.30) and (2.31) hold, then for the good iterates, $j \in J$, the search direction dj is a strong direction of descent for the $t\backslash$ merit function in the sense that the first order reduction is proportional to the KKT error.

We will choose C* so that (2.30) holds for *all* iterations. To see how to do this we note from (2.10) that

$$p_Z = -B_k^{-} \; g_k - \zeta_k D_k \; w_k,$$

so that for j = A; (2.30) can be written as

$$\zeta_k[2\cos\theta_k|g_k^T Z_k w_k| + w_k^T B_k^{-x} Z \; g_k + CkV\$BZ^l w_k] \leq p\|c_k h. \qquad (2.33)$$

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

$$a = \min\{1, \&\} \qquad (2.34)$$

where $\hat{\zeta}_k$ is the largest value that satisfies (2.33) as an equality.

The penalty parameter p_k must satisfy (2.31), so we define it at every iteration of the algorithm by

$$\mu_k = \begin{cases} w - i & \text{if Mfc-i} \geq \|\lambda_k\|_\infty + 2\rho \\ P^*\|oo + 3p & \text{otherwise.} \end{cases} \qquad (2.35)$$

The damping factor 0b and the updating formula for the penalty parameter fi_k have been defined so as to give strong descent for the good iterates J. We now show that they ensure that the search direction is also a direction of descent (but not necessarily of strong descent) for the other iterates, $k \notin J$. Since (2.30) holds for all iterations by our choice of £fc, we have in particular

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

Using this and (2.35) in (2.27), we have

$$D\phi_{\mu_k}(x_k; d_k) \leq -\|Z_k^T g_k + \zeta_k w_k\| \, \|p_z\| \cos\theta_k \text{ -pk\\ck\\i.} \tag{2.36}$$

The directional derivative is thus non-positive. Furthermore, since *Wk* = 0 whenever *Ck* = 0, it is easy to show that this directional derivative can only be zero at a stationary point of problem (1.1)-(1.2). Note, as shown in (Biegler et al (1996)) that the condition on *pk* can also be replaced by a weaker condition:

$$\mu_k \|c_k\| \text{i} > \text{\\giYpy\\} \tag{2.37}$$

and the same results hold, without calculation of the multipliers.

2.3. The Algorithm

We can now give a complete description of the algorithm that incorporates all the ideas discussed so far, and that specifies when to apply finite differences to approximate the cross term. The idea is to consider the relative sizes of p_Y and p_z. Update Criterion I generates the three regions i2i,i?2 and *R$* as shown in (Biegler et al (1995)). The algorithm starts by calculating p_Y and p_z with *Wk* = $\overline{W}k$ = 0. If the search direction is in iJi, we proceed. Otherwise we recompute *Wk* by finite differences, use this value to recompute p_z, and proceed. The reason for applying finite differences in this fashion is that in the regions *R2* and *R3* the convergence path is not sufficiently tangential to the constraints to give a superlinear step. Therefore we need to resort to finite differences to obtain a good estimate of *w^*. The motivation behind this strategy will become clearer when we study the rate of convergence of the algorithm in §5.

Note from Updating Criterion I that the BFGS update of *Bk* is skipped if the search direction is in *R$*. A precise description of the algorithm follows.

Algorithm I

1. Choose constants *q e* (0,1/2), *p* > 0 and *T,T** with 0 < r < r' < 1, and 7_{fd} > 0 for (2.16). For (2.15), select a summable sequence of positive numbers {7*}. Set *k* := 1 and choose a starting point *x*, an initial value *p.* for the penalty parameter, an (n - *m)* x (n - m) symmetric and positive definite starting matrix *B*.

2. Evaluate /*,£*,<* and J4*, and compute V* and Z*.

3. Set *findiff* = *false*, *Wk* = ŧU* = 0 and compute p_Y by solving the system

$$(AlYk)p_Y = -c^*. \qquad \text{(range space step)} \tag{2.38}$$

4. Compute p_z from

$$BkPz = -Z]z9k- \qquad \text{(null space step)} \tag{2.39}$$

5. If (2.15) is *not* satisfied and *<7k _< S,* a preset tolerance, set *findiff* = *true* and recompute *Wk* from equation (1.18) or (1.19).

6. *If findiff* = *true* use this new value of *Wk* to choose the damping parameter (* from equations (2.33) and (2.34) and recompute p_z from equation (2.10).

7. Define the search direction by

$$d_k = Y_{kPY} + Z_k p_z, \tag{2.40}$$

and set $a_k = 1$.

8. Test the line search condition

$$\text{tfVijb}(^{x*} + {}^a k^d k) < \leq t > n_k(**) + V<*kD<f>n_k\{x_k; d_k). \tag{2.41}$$

9. If (2.41) is not satisfied, choose a new a* € $[ra_k, T^l a_k]$ and go to 9; otherwise set

$$x_{k+x} = x_k + a_k d_k. \tag{2.42}$$

10. Evaluate /*+ii0*+i>^{c}*+ii A_{k+U} and compute Y_{k+X} and Z_{fc+}i-

11. Compute the Lagrange multiplier estimate

$$\mathbf{A^{*+}i} = -[Y\wedge A\wedge r'Y\wedge g\wedge u \tag{2.43}$$

and update fi_k so as to satisfy (2.35).

12. *Ufindiff = true* calculate $\overline{w}_k$ by (2.7) or (2.8).

13. If $s\wedge y_k \leq 0$ or if (2.16) is not satisfied, set £fc+i = B_k. Else, compute

$$s_k = a_k pz, \tag{2.44}$$

$$\mathbf{y_k = zZ\backslash yL\{x_{k+u}\backslash_M) - VL(x^*, A_{fc+}i)] - W_{fc}} \tag{2.45}$$

and compute £fc+i by the BFGS formula (2.9).

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

In the next sections we present several convergence results for Algorithm I. The analysis, which does not assume that the BFGS matrices B_k are bounded, is based on the results of Byrd and Nocedal (1991), who have studied the convergence of the Coleman-Conn updating algorithm. We also make use of some results of Xie (1991), who has analyzed the algorithm proposed by Nocedal and Overton (1985) using non-orthogonal bases *Y* and *Z*. The main difference between this paper and that of Xie stems from our use of the correction terms w_k and $\overline{w}_k$, which are not employed in his method.

3. Semi-Local Behavior of the Algorithm.

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

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

(I) The functions / : $R^n \to R$ and c : $R^n \to R^m$ 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 e D, and there exist constants 70 and Po such that

$$\|Y(x)[A(x)^T Y(x)]^{-1}\| \leq 70, \qquad ||Z(*)|| \leq A), \tag{3.1}$$

for all x e D.

(III) The correction term Wk is chosen so that there is a constant $K > 0$ such that for all

$$\text{IKII} \leq {}^*\text{I|c*||.} \tag{3.2}$$

(IV) For all $k \geq 1$ for which B_k is updated, (2.18) and (2.19) hold.

Note that condition (I) is rather strong, since it would often be satisfied only if D is bounded, and it is far from certain that the iterates will remain in a bounded set. Nevertheless the convergence result of this section can be combined with the local analysis of §4 to give a satisfactory semi-global result. Condition (II) requires that the basis matrices Y and Z be chosen carefully, and is important to obtain good behavior in practice. Note that (3.1) and (2.38) imply that

$$\text{||nPY|j} \leq \text{7ol|c*||.} \tag{3.3}$$

Relation (3.2) holds for the finite difference approach, since (1.18) implies that $w_k = O(YkP_Y)$, and since (I) ensures that {||cfc||} is uniformly bounded (see (4.19)). Condition (IV) is justified in the last paragraphs of §2.1, where it is shown that (2.18) and (2.19) are satisfied whenever BFGS updating takes place in a neighborhood of a solution point. Condition (IV) and Theorem 2.1 ensure that at least half of the iterates at which BFGS updating takes place are good iterates. The following result concerns the good iterates J, as given in Definition 2.1.

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

$$\phi_\mu(x_j) - \phi_\mu(x_{j+1}) \geq \gamma_\mu \left[\|Z_j^T g\text{ill}^2 + \text{IMIi}\right] \bullet \tag{3.4}$$

Proof. Follows exactly as in (Biegler et al (1995))

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* {/i*} *are constant for all sufficiently large k and*

$$\liminf_{k\to\infty}(\|Z_k^T g_k\| + \|c_k\|) = 0.$$

Proof. Follows exactly as in (Biegler et al (1995))

4. 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 /i* is chosen large enough, then Z* is a point of attraction for the sequence of iterates {z*} 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.

$$G_k = Z^*[V^2_{xx}L(x_{ky}\backslash_k)Z_k. \qquad (4.1)$$

Assumptions 4.1 The point $x+$ is a local minimizer for problem (1.1)-(1.2) at which the following conditions hold.

(1) The functions / : R^n -* R and c : R^n -+ R^m 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* G R^m such that

$$VL(x^*, A^*) = g(x^*) + A(x^*)\backslash_m = 0.$$

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

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

$$\backslash\backslash Y(x)[A(x)^T Y(x)]^{-l}\backslash\backslash < Z0, \qquad ||Z(*)|| \leq A), \qquad (4.2)$$

and

$$||[y(x)Z(x)]^{-1}|| \leq 7c. \qquad (4.3)$$

(5) $Z(x)$ and $X(x)$ are Lipschitz continuous in a neighborhood of rr*, i.e. there exist constants y_z and 7A such that

$$\|\lambda(x) - \lambda(z)\| \leq \gamma_\lambda \|x - * II, \qquad (4.4)$$
$$\backslash\backslash Z(x) - Z(z)\backslash\backslash \leq y_t\backslash\backslash x-z\backslash\backslash, \qquad (4.5)$$

for all x,z near x».

Note that (1), (3) and (5) imply that for all (x,A) sufficiently near (x,,A,), and for all q e R^n-^{m},

$$m|M|^2 \leq_9 {}^r C?(x,A)_9 \leq M||_g||^2, \qquad (4.6)$$

for some positive constants m,M. We also note that Assumptions 4.1 ensure that the conditions (2.18)-(2.19) required by Theorem 2.1 hold whenever BFGS updating takes place in a neighborhood of x^*_y as argued at the end of §3.3. Therefore Theorem 2.1 can be applied in the convergence analysis.

The following two lemmas are proved by Xie (1991) for very general choices of Y and Z. Their result generalizes Lemmas 3.1 and 4.2 of Byrd and Nocedal (1991); see also Powell (1978).

Lemma 4.1 *If Assumptions J^.l hold, then for all x sufficiently near x+*

$$\text{Till}^* - x.\backslash\backslash \leq ||c(x)|| + \backslash\backslash Z\{x)^T g\{x)\backslash\backslash \leq {}_{72}||x - x,||, \qquad (4.7)$$

for some positive constants 71,72-

This result states that, near a;*, 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 4.2 *Suppose that Assumptions 4-1 hold at* x_m. *Then for any fi* > ||A«||oo *there exist constants* 73 > 0 *and* 74 > 0, *such that for all x sufficiently near* x«

$$73\|x - x.\|^2 \leq 4,(x) - *_{„}(«.) \leq 74 \; [\|Z(z)^T 0(z)\|^2 + H*)h] \bullet \qquad (4\text{-}8)$$

Note that the left inequality in (4.8) implies that for a sufficiently large value of the penalty parameter, the merit function will have a strong local minimizer at 2*. 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 z». To rule this out we make the following assumption.

Assumption 4.2 The line search has the property that, for all large *k*, ^((1 — *0)xk* + 0£fc+i) < *<f>n{xk)* for all *0* ***e*** [0,1]. In other words, *Xk+i* is in the connected component of the level set *{x* : $<£_M(x)$ < *<f>*$n(x_k)$*}* that contains x_k.

There is no practical line search algorithm that can guarantee this condition, but it is likely to hold close to rr«. Assumption 4.2 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 updates for equality constrained optimization.

Lemma 4.3 *Suppose that the iterates generated by Algorithm I are contained in a convex region D satisfying Assumptions 3.1 If an iterate* x_{ko} *is sufficiently close to a solution point x* that satisfies Assumptions 4-1, and if the weight* fi_{ko} is *large enough, then the sequence of iterates converges to x+.*

Proof. Follows exactly as in (Biegler et al (1995)).

4.1. R-Linear Convergence.

For the rest of the paper we assume that the iterates generated by Algorithm I converge to 2*, which implies that for all large A; /z* = *fi* > ||A,||. 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,

$$U = \{k : B_{k+1} = BFGS(B_k, s_k, y_k)\}, \qquad (4.9)$$

and let

$$\% = \text{tfn}\{1, 2, ..., *\}. \qquad (4.10)$$

The number of elements in U_k will be denoted by $\backslash U_k \backslash$.

Theorem 4.4 *Suppose that the iterates* $\{x_k\}$ *generated by Algorithm I converge to a point* x, *that satisfies Assumptions 4-1- Then for any k eU and any j >k*

$$\|x_j - x_*\| \leq C r^{|U_k|}, \qquad (4.11)$$

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

Proof. Follows exactly as in (Biegler et al (1995)).

This result implies that if {|£/*!/&} 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 *\Uk\/k* -> 0. We therefore need to examine the iteration more closely.

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

$$\psi(B) = tr(B) - \ln(\det(B)), \tag{4.12}$$

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

$$\ln \text{cond}(B) < \psi(B), \tag{4.13}$$

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

$$\tilde{y}_k = G_*^{-1/2} y_k, \qquad \tilde{s}_k = G_*^{1/2} s_k, \tag{4.14}$$

$$\tilde{B}_k = G_*^{-1/2} B_k G_*^{-1/2}, \tag{4.15}$$

$$\cos\tilde{\theta}_k = \frac{\tilde{s}_k^T \tilde{B}_k \tilde{s}_k}{\|\tilde{B}_k \tilde{s}_k\| \|\tilde{s}_k\|} \tag{4.16}$$

and

$$\tilde{q}_k = \frac{\tilde{s}_k^T \tilde{B}_k \tilde{s}_k}{\tilde{s}_k^T \tilde{s}_k}. \tag{4.17}$$

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

$$\begin{aligned}\psi(\tilde{B}_{k+1}) &= \psi(\tilde{B}_k) + \frac{\|\tilde{y}_k\|^2}{\tilde{y}_k^T \tilde{s}_k} - 1 - \ln \frac{\tilde{y}_k^T \tilde{s}_k}{\tilde{s}_k^T \tilde{s}_k} + \ln\cos^2\tilde{\theta}_k \\ &\quad + \left[1 - \frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k} + \ln\frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k}\right].\end{aligned} \tag{4.18}$$

This expression characterizes the behavior of the BFGS matrices *'Bk,* 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 *Wk* and tUjt, these are accurate to second order.

Lemma 4.5 *// at the iterate Xk, the corrections Wk and Wk are computed by the finite difference formulae (1.18)-(2.7) or (1.19)-(2.8)f and ifxk is sufficiently close to a solution point* x* *that satisfies Assumptions 4-1, then*

$$w_k = O(\|p_Y\|), \tag{4.19}$$

$$\|w_k - Z_*^T W_* Y_k p_Y\| = O(\sigma_k \|p_Y\|) \tag{4.20}$$

and

$$\|\bar{w}_k - Z_k^T W_* Y_k p_Y\| = O(\sigma_k \|p_Y\|). \tag{4.21}$$

Proof. The proof for the formulae (1.18)-(2.7) follow exactly as in (Biegler et al (1995)), while the proof for the formulae (1.19)-(2.8) follow exactly as in (Biegler et al (1996)).

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

Theorem 4.6 *Suppose that the iterates {xk} generated by Algorithm I converge to a solution point x+ that satisfies Assumptions 4.1. Then* {||£*||} *and* {H-B^1!!} *are bounded, and for all k €U*

$$\mathbf{11(5^* - Z?W.Z.)p_z\backslash\backslash = o(\|<f^*\|).} \tag{4.22}$$

Proof. Here we consider only the definition of y_k using (2.5). A similar proof using (2.6) follows along the lines shown in (Biegler et al, **1996).** We will only consider iterates k for which BFGS updating of B_k takes place. We have from (2.45), (2.42), (2.40), (2.13) and (2.44)

$$\begin{aligned} y_k &= Z_k^T[\nabla L(x_{k+1}, \lambda_{k+1}) - \nabla L(x_k, \lambda_{k+1})] - \overline{w}_k \\ &= Zj \left[\int_0^1 V^2_{xx}L\{x_k + Ta_kd_k, A^*_{+1})<fTJ\right] a_kd_k - \overline{w}_k \\ &= \alpha_k Z_k^T \tilde{W}_k (Z_k p_Z + Y_k p_Y) - \overline{w}_k \\ &= Z_k^T \tilde{W}_k Z_k s_k + \alpha_k (Z_k^T \tilde{W}_k - Z_*^T W_*) Y_k p_Y + (\alpha_k Z_*^T W_* Y_k p_Y - \overline{w}_k). \end{aligned} \tag{4.23}$$

Since $\overline{w}_k$ is either zero or computed by finite differences, we need to consider these two cases separately.

Part I. Let us first assume that *Wk* is zero. A simple computation shows that $\|Z_k^T \tilde{W}_k - Z_*^T W_*\| = O(a_k)$. Using Assumptions 4.1 in (4.23) we have

$$\begin{aligned} y_k &= Z_k^T \tilde{W}_k Z_k s_k + (\sigma_k + 1) O(\alpha_k \|p_Y\|) \\ &= (Z_k^T \tilde{W}_k Z_k - G_*) s_k + G_* s_k + (\sigma_k + 1) O(\alpha_k \|p_Y\|). \end{aligned} \tag{4.24}$$

Recalling (4.14) and noting that ỹ^S̃k = *yjsk* we have

$$\hat{y}j\tilde{s}^* = s^T{}_k(Zl\bar{W}_kZ_k - G,)s_k + \backslash\backslash\tilde{s}_kf + (<r^* + 1)O(\alpha_k\|p_Y\|)\|\bar{s}_k\|,$$

since ||s"fc|| and ||s*|| are of the same order. Therefore

$$\begin{aligned} \frac{\tilde{y}_k^T \tilde{s}_k}{\|\bar{s}_k\|^2} &= 1 + \frac{s_k^T (Z_k^T \tilde{W}_k Z_k - G_*) s_k}{\|\bar{s}_k\|^2} + (\sigma_k + 1) O\left(\frac{\|\alpha_k p_Y\|}{\|\bar{s}_k\|}\right) \\ &= 1 + O(\sigma_k) + (\sigma_k + 1) O\,(\wedge\wedge) \end{aligned} \tag{4.25}$$

Similarly from (4.24) and (4.14) we have

$$\begin{aligned} f_k y k \;\_< \;& \backslash\tilde{\backslash}\{zlw_kz_k\text{-}G.\wedge lfllG;^1!! + 2\backslash\backslash\{zl\tilde{w}_kz_k\text{-}G.)s_k\backslash\backslash \; \|GT^{1/2}\| \; p_{fc}\| + p_{fc}\|^2 \\ & +2(a_k + l)O(\|a_{fc}p_Y\|)\|G;5\| \; (p^*\| + \backslash\backslash\{\bar{Z}lW_kZ_k - G.)s_k\backslash\backslash\backslash\backslash G:^{1/2}\backslash\backslash) \\ & +(\sigma_k + l)^2O(\|a_{fcPY}\|)^2, \end{aligned}$$

and thus

$$\frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} \le 1 + O(\sigma_k) + (1+\sigma_k)^2 O\left(\frac{\|\alpha_k p_Y\|}{\|\tilde{s}_k\|}\right) \tag{4.26}$$

At this point we invoke the update criterion, and note from (2.15) that if BFGS updating of B_k takes place at iteration k, then $\|\alpha_k p_Y\| \le \gamma_k \|s_k\|$ where $\{\gamma_k\}$ is summable. Using this, the assumption that α_k converges to zero, and (4.25) we see that for large k

$$\frac{\tilde{y}_k^T \tilde{s}_k}{\|\tilde{s}_k\|^2} = 1 + O(\sigma_k + \gamma_k), \tag{4.27}$$

and using (4.26)

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

Therefore

$$\frac{\|\tilde{y}_k\|^2}{\tilde{y}_k^T \tilde{s}_k} = \frac{\|\tilde{y}_k\|^2}{\|\tilde{s}_k\|^2} \frac{\|\tilde{s}_k\|^2}{\tilde{y}_k^T \tilde{s}_k} = 1 + O(\sigma_k + \gamma_k). \tag{4.28}$$

We now consider $\psi(\tilde{B}_{k+1})$ given by (4.18). A simple expansion shows that for large k, $\ln(1 + O(\sigma_k + \gamma_k)) = O(\sigma_k + \gamma_k)$. Using this, (4.27) and (4.28) we have

$$\psi(\tilde{B}_{k+1}) = \psi(\tilde{B}_k) + O(\sigma_k + \gamma_k) + \ln\cos^2\tilde{\theta}_k + \left[1 - \frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k} + \ln\frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k}\right]. \tag{4.29}$$

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

$$\psi(\tilde{B}_{k+1}) \le \psi(\tilde{B}_k) + O(\sigma_k + \gamma_k). \tag{4.30}$$

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

Part II. Let us now consider the iterates k for which updating takes place and for which $\bar{w}_k$ is computed by finite differences. In this case (2.16) holds. Again we begin by considering (4.23),

$$y_k = Z_k^T \tilde{W}_k Z_k s_k + \alpha_k (Z_k^T \tilde{W}_k - Z_k^T W_*) Y_k p_Y + (\alpha_k Z_k^T W_* Y_k p_Y - \bar{w}_k).$$

Using (4.21) the last term is of order $O(\sigma_k \alpha_k \|p_Y\|)$ and so is the second term. Thus

$$\begin{aligned} y_k &= Z_k^T \tilde{W}_k Z_k s_k + O(\sigma_k \alpha_k \|p_Y\|) \\ &= (Z_k^T \tilde{W}_k Z_k - G_*) s_k + G_* s_k + O(\sigma_k \alpha_k \|p_Y\|). \end{aligned} \tag{4.31}$$

Noting that $\tilde{y}_k^T \tilde{s}_k = y_k^T s_k$ and recalling the definition (4.14) we have

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

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

$$\begin{aligned} \frac{\tilde{y}_k^T \tilde{s}_k}{\|\tilde{s}_k\|^2} &= 1 + \frac{s_k^T (Z_k^T \tilde{W}_k Z_k - G_*) s_k}{\|\tilde{s}_k\|^2} + O\left(\sigma_k \frac{\|\alpha_k p_Y\|}{\|\tilde{s}_k\|}\right) \\ &= 1 + O(\sigma_k) + O\left(\sigma_k \frac{\|\alpha_k p_Y\|}{\|\tilde{s}_k\|}\right). \end{aligned} \tag{4.32}$$

Similarly from (4.31) and (4.14) we have

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

and thus

$$\frac{\|\tilde y_k\|^2}{\|\tilde s_k\|^2} \le 1 + O(\sigma_k) + \sigma_k O\left(\frac{\|\alpha_k p_Y\|}{\|\tilde s_k\|}\right) + \sigma_k^2 O\left(\frac{\|\alpha_k p_Y\|^2}{\|\tilde s_k\|^2}\right). \qquad (4.33)$$

We now invoke Update Criterion I, and note from (2.16) that if BFGS updating of B_k takes place at iteration k, then $\|p_Y\| \le \gamma_k \|p_Z\| / \sigma_k^{1/2}$. Using this, (4.32) and the fact that σ_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 (4.33)

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

Therefore

$$\frac{\|\tilde y_k\|^2}{\tilde y_k^T \tilde s_k} = \frac{\|\tilde y_k\|^2 / \|\tilde s_k\|^2}{\tilde y_k^T \tilde s_k / \|\tilde s_k\|^2} = 1 + O(\sigma_k^{1/2}). \qquad (4.34)$$

We now consider $\psi(\tilde B_{k+1})$ given by (4.18). Noting that $\ln(1 + O(\sigma_k^{1/2})) = O(\sigma_k^{1/2})$ for all large k, we see that if updating takes place at iteration k

$$\psi(\tilde B_{k+1}) = \psi(\tilde B_k) + O(\sigma_k^{1/2}) + \ln\cos^2\tilde\theta_k + \left[1 - \frac{\tilde q_k}{\cos^2\tilde\theta_k} + \ln\frac{\tilde q_k}{\cos^2\tilde\theta_k}\right]. \qquad (4.35)$$

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

$$\psi(\tilde B_{k+1}) \le \psi(\tilde B_k) + O(\sigma_k^{1/2}). \qquad (4.36)$$

We now combine the results of Parts I and II of this proof. Let us subdivide the set of iterates U for which BFGS updating takes place into two subsets: U' corresponds to the iterates in which $\bar w_k = 0$, and U'' to the iterates in which finite differences are used. We also define $U'_k = U' \cap \{1,2,\dots,k\}$ and $U''_k = U'' \cap \{1,2,\dots,k\}$.

Summing over the set of iterates in U_k, using (4.30) and (4.36), and noting that $\tilde B_{j+1} = \tilde B_j$ for $j \notin U_k$, we have

$$\psi(\tilde B_{k+1}) \le \psi(\tilde B_1) + C_1 \sum_{j\in U''_k} \sigma_j^{1/2} + C_2 \sum_{j\in U'_k} \sigma_j + C_3 \sum_{j\in U'_k} \gamma_j, \qquad (4.37)$$

for some constants $Ci, C_2, C\$$. By (4.11) and since $\backslash U![\backslash \leq \backslash Uj\backslash$,

$$\sum_{j\in U''} a_j T \wedge \sum_{j\in U''} C^{1/2}r^{|U_j|/2}$$

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

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

$$< \infty.$$

Similarly

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

and since $\{7^*\}$ is summable we conclude from (4.37) that $\{i/)(\tilde{B}_k)\}$ is bounded above. By (4.12) $t/j\{\tilde{B}_k) = 5Z?=i(\wedge t \sim\sim \text{Ini}^*)$, where $l\{$ are the eigenvalues of $\tilde{£}?^*$, and it is easy to see that this implies that both $\|2?fc\|$ and HB^H are bounded.

To prove (4.22), we sum relations (4.29) and (4.35), recalling that o^, 7^ and a^¯ are summable, to obtain

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

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

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

and

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

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

$$\lim_{\substack{k\to\infty \\ k\in U}} \cos\tilde{\theta}_k = \lim_{\substack{k\to\infty \\ k\in U}} \tilde{q}_k = 1. \qquad (4.38)$$

Now from (4-16)-(4.17)

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

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

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

It is clear from (4.38) that the last term converges to 0 for $k \in U$, which implies that (4.22) holds.

□

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

Theorem 4.7 *Suppose that the iterates $\{x_k\}$ generated by Algorithm I converge to a solution point x^* that satisfies Assumptions 4-1- Then the rate of convergence is at least R-linear.*

Proof. Theorem 4.6 implies that the condition number of the matrices {J3*} is bounded. Therefore *all* the iterates are good iterates, and reasoning as in the proof of Theorem 4.4 we conclude that for all j

$$\|x_j - x_*\| \leq Cr^j,$$

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

D

5. Superlinear Convergence

Without the correction terms w_k and $\overline{w}_k$, 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 assuming that a good starting matrix $B\backslash$ is used. This result has been extended by Xie (1991) for more general bases and for any starting matrix $B\backslash > 0$. In this section we will show that if the correction terms are used in Algorithm I, the rate of convergence is 1-step Q superlinear. This result is possible by Update Criterion I and by the selected application of finite difference approximations, which allow BFGS updating to occur more frequently.

Of course, to establish superlinear convergence we need to ensure that the steplengths a_k have the value 1 for all large k. 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. There are a number of stepsize strategies (e.g., Watchdog, second order corrections) that will ensure unit steps near the solution. We begin by showing that the damping parameter **Ofc;** used in (2.39) to ensure that descent directions are always generated, has the value of 1 for all large A;

We have shown in Theorem 5.6 that H-B^*1!! is bounded above. Also (4.19), (4.2) and (2.38) show that, when finite differences are used, w_k = O(||p$_Y$||) = OflkkH). Noting that II • I_L< II • 111, we therefore see that there is a constant C such that the left hand side of (2.33) can be bounded by

$$\zeta_k[2\cos\theta_k|g_k^T Z_k w_k| + w_k^T B_k^{-1} Z_k^T g_k + \zeta_k w_k^T B_k^{-1} w_k] \leq [\zeta_k C(\|e_k\| + \zeta_k\|c_k\|)]\|c_k\|_1,$$

since $g\%Z_k$ = 0(||eik||). As the iterates converge to the solution, and since $(_k \leq 1$, the term inside the square brackets is less than the constant p given in (2.33), showing that C* = 1 for all large k. This, and the remarks made at the end of §4 show that all the safeguards included in Algorithm I become inactive asymptotically.

The accuracy of w_k and B_k in a neighborhood close to the solution lead to the following lemma, which is an application of the well-known result of Boggs, Tolle and Wang (1982).

Lemma 5,1 *Suppose that the iterates generated by Algorithm I converge R-linearly to a point x+ that satisfies Assumptions 4.1, and that* $a_k = 1$ *for all large k. If, in addition*

$$\lim_{k\to\infty} \frac{\|B_k p_Z + w_k - Z_*^T W_* d_k\|}{\|d_k\|} = 0, \tag{5.1}$$

then the rate of convergence is l-step Q-superlinear.

Proof. The proof follows exactly as in (Biegler et ai (1995)).

We can now prove the final result of this section. The analysis is complicated by the fact that BFGS updating may not always take place, and by the fact that the correction terms are sometimes computed by finite differences. We therefore consider the following three sets of iterates, based on Update Criterion I and illustrated in Figure 2.

- $R_1 = \{j| \, \|p_Y^{(j)}\| \le \gamma_j \|p_Z^{(j)}\|\}$,
- R_2 = {*j i* R_X | $\|p_Y^{(j)}\| \le \|p_Z^{(j)}\|/\sigma_j^{1/2}\}$,
- $R_3 = \{j| \|p_Y^{(j)}\| > \|p_Z^{(j)}\|/\sigma_j^{1/2}\}$,

and note that both 7* and a* are summable.

Theorem 5.2 *Suppose that the iterates generated by Algorithm I converge R-linearly to a point x* that satisfies Assumptions 4 1, and that* $a_k = 1$ *for all large k. Then the rate of convergence is l-step Q-superlinear.*

Proof. Since d* = *YkP*$_Y$ + *ZkPz* we have

$$\begin{bmatrix} p_Y \\ p_Z \end{bmatrix} = [Y_k \; Z_k]^{-1} d_k.$$

Therefore assumption (4.3) implies that

IIPvll = O(||d$_{fc}$||), IIPzll = 0(11411). (5.2)

Now

$$\begin{aligned} \|B_k p_Z + w_k - Z_*^T W_* d_k\| &\le \|B_k p_Z - Z_*^T W_* Z_k p_Z\| + \|w_k - Z_*^T W_* Y_k p_Y\| \\ &\le \|B_k p_Z - Z_*^T W_* Z_* p_Z\| + \|w_k - Z_*^T W_* Y_k p_Y\| \\ &\quad + O(\|e_k\| \|p_Z\|). \end{aligned}$$

Since by (5.2) the last term is of order o(||p$_z$||) = o(||rf/t||), the objective of the proof is to show that

B$_{kPz}$ - *%W.Z.p*$_{\%}$\\ + *w*$_k$ - *fiW.YkpyW* = o(||4||), (5.3)

for this together with (5.1) will give the desired result. We consider the three regions i?i,i?2 and H3 separately. Algorithm I is designed so that in *R2* and #3, w_k must be computed by finite differences. On the other hand since p_z is recomputed in step 7, after which we can be in any of the three regions, we see that in i?i, w_k = o(||p$_Y$||).