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(5.23) uses (5.17), which follows from the 1,2 block of (5.9), namely (4.8). We now use a similar argument to simplify the quadratic term in (5.39). Instead of (4.8), we have, from the 1,2 block of (5.40),

$$-\widehat{Q}_1^T[A_x(\widehat{x})\{\overline{x}-x^*\}]\widehat{Q}_2-\widehat{\Lambda}_1\{\Delta Y-\widehat{Y}^*\}_{12}+\{\Delta Y-\widehat{Y}^*\}_{12}\widehat{\Lambda}_2=O(\|\widehat{x}-x^*\|^2).$$

Instead of (5.17), we conclude that

$$[\widehat{F}_{YY}(\widehat{Z})\{\Delta Y-\widehat{Y}^*\}\{\Delta Y-\widehat{Y}^*\}]_{11}+[\widehat{F}_{xY}(\widehat{Z})\{\overline{x}-x^*\}\{\Delta Y-\widehat{Y}^*\}]_{11}$$
$$=O(\|\widehat{x}-x^*\|^2\|\Delta Y-\widehat{Y}^*\|).$$

Again using (5.40) to define $\Delta Y-\widehat{Y}^*$ in terms of the x and ω components of $\overline{Z}-\widehat{Z}^*$, we see that the right-hand side consists of two terms, of which one can be absorbed into the first term of (5.41), and the other into the second. We therefore see that, just as the quadratic form in (5.8) reduces to that in (5.23), the quadratic form in (5.39) reduces to

$$\psi+\widetilde{h}\cdot\begin{bmatrix}\widehat{\lambda}_1+\Delta\omega-\lambda_1^*\\ \overline{x}-x^*\end{bmatrix}+\tfrac{1}{2}\{\overline{x}-x^*\}^T\widehat{W}\{\overline{x}-x^*\} \tag{5.42}$$

where $\widetilde{h}=O(\|\widehat{x}-x^*\|^2)$. The constraint (5.40) reduces to (4.17), i.e.

$$\widehat{K}\begin{bmatrix}\widehat{\lambda}_1+\Delta\omega-\lambda_1^*\\ \overline{x}-x^*\end{bmatrix}=O(\|\widehat{x}-x^*\|^2). \tag{5.43}$$

The optimality conditions for the quadratic program defined by (5.42)–(5.43) are

$$\begin{bmatrix}\begin{bmatrix}0&0\\0&\widehat{W}\end{bmatrix}&-\widehat{K}^T\\ \widehat{K}&0\end{bmatrix}\begin{bmatrix}\begin{bmatrix}\widehat{\lambda}_1+\Delta\omega-\lambda_1^*\\ \overline{x}-x^*\end{bmatrix}\\ \text{vec }\{\overline{U}_{11}-\widehat{U}_{11}^*\}\end{bmatrix}=O(\|\widehat{x}-x^*\|^2), \tag{5.44}$$

By assumption, K^* has full rank and (5.31) is positive definite, so

$$\begin{bmatrix}\begin{bmatrix}0&0\\0&W^*\end{bmatrix}&\{K^*\}^T\\ K^*&0\end{bmatrix}$$

is nonsingular. Therefore, using (4.18)–(4.19) and noting that $\|\widehat{W}-W^*\|$ $=O(\|\widehat{x}-x^*\|)$, we see that the inverse of the coefficient matrix of (5.44) is bounded for $\widehat{x}$ near x^*. The desired quadratic contraction is therefore proved. ∎

with the understanding that all Y_{11} terms are omitted. The $O(\|\hat{x} - x^*\|^2)$ term on the right-hand side is justified by (3.27) and (5.33).

The necessary condition for a pair $\Delta Z, \Delta U$ to solve the quadratic program defining a step of Iteration 3 is, in addition to the constraints (5.9)–(5.10), that there exists a dual matrix ΔU such that

$$\Delta U : \hat{F}_Z(\hat{Z}) = \hat{L}_Z(\hat{Z}, \hat{U}) + [\hat{L}_{ZZ}(\hat{Z}, \hat{U})\Delta Z]. \tag{5.37}$$

where rows and columns of the coefficient matrix corresponding to Y_{11} have been omitted because of (5.10). Noting that $\Delta Z = \overline{Z} - \hat{Z}$ and subtracting (5.36) from (5.37) gives

$$[\hat{L}_{ZZ}(\hat{Z}, \hat{U})\{\overline{Z} - \hat{Z}^*\}] - \{\overline{U} - \hat{U}^*\} : \hat{F}_Z(\hat{Z}) = O(\|\hat{x} - x^*\|^2), \tag{5.38}$$

where $\overline{U} = \hat{U} + \Delta U$.

Equations (5.35),(5.38) state the first-order optimality conditions for the quadratic program

$$\min_{\overline{Z} - \hat{Z}^*} \quad h \cdot \{\overline{Z} - \hat{Z}^*\} + \tfrac{1}{2}[\hat{L}_{ZZ}(\hat{Z}, \hat{U})\{\overline{Z} - \hat{Z}^*\}\{\overline{Z} - \hat{Z}^*\}] \tag{5.39}$$

$$\text{subject to} \qquad [\hat{F}_Z(\hat{Z})\{\overline{Z} - \hat{Z}^*\}] = O(\|\hat{x} - x^*\|^2) \tag{5.40}$$

where the first term in (5.39) is an inner product, with h (which has the same structure as Z) satisfying $h = O(\|\hat{x} - x^*\|^2)$. It is understood that there are no Y_{11} terms in $\overline{Z}$, $\hat{Z}^*$. Note that the Hessian and constraint coefficients of this quadratic program are identical to those of (5.8)–(5.9). We shall now simplify this quadratic program, using an argument similar to that which reduced (5.8)–(5.9) to (5.23)–(5.24). First consider the linear term in (5.39). We have

$$h \cdot \{\overline{Z} - \hat{Z}^*\} = \tilde{h} \cdot \begin{bmatrix} \hat{\lambda}_1 + \Delta\omega - \lambda_1^* \\ \overline{x} - x^* \end{bmatrix} + \psi \tag{5.41}$$

where $\tilde{h} \in \Re^{m+1}$ and $\psi \in \Re$ satisfy $\tilde{h} = O(\|\hat{x} - x^*\|^2)$ and $\psi = O(\|\hat{x} - x^*\|^4)$. This equation holds because of the constraint (5.40), which defines the Y and Θ elements of $\overline{Z} - \hat{Z}^*$ in terms of the x and ω components, by analogy with (4.8)–(4.10). Now consider the quadratic term in (5.39). The argument that showed that the quadratic form in (5.8) reduces to that in

We are now ready to prove the main convergence theorem.

Theorem 5.4 *Suppose that K^* has independent rows and that the reduced Hessian (5.31) is positive definite. Then there exist constants ϵ and C such that, if $\|\widehat{x} - x^*\| \leq \epsilon$, then*

$$\|\overline{x} - x^*\| \leq C\|\widehat{x} - x^*\|^2$$

for both Iterations 3 and 4. Consequently, both iterations generate points $\widehat{x}$ which converge quadratically to the solution x^*.

Proof: From Theorem 5.3, assuming that $\widehat{x}$ is sufficiently close to x^*, a necessary condition for a pair $\widehat{Z}^*, \widehat{U}^*$ to solve the nonlinear program (3.11)–(3.12) (*without* the condition $Y_{11} = 0$ imposed), is that, in addition to (3.12), the equation (5.32) holds. Theorem 3.1 shows that we can take the $\widehat{Y}^*$ component of $\widehat{Z}^*$ to satisfy $\|\widehat{Y}^*\| = O(\|\widehat{x} - x^*\|)$ and $\|\widehat{Y}^*_{11}\| = O(\|\widehat{x} - x^*\|^2)$. Furthermore, we can expand $\widehat{F}$ in a Taylor series just as in the proof of Theorem 4.2, obtaining all of equations (4.13)–(4.16) exactly as before, the only difference being that these equations are not square systems. Specifically, (4.16), with its Y_{11} terms absorbed into the right-hand side, gives

$$[\widehat{F}_Z(\widehat{Z})\{\overline{Z} - \widehat{Z}^*\}] = O(\|\widehat{x} - x^*\|^2). \tag{5.35}$$

Now let us expand (5.32) in a Taylor series. We have

$$0 = \widehat{L}_Z(\widehat{Z}^*, \widehat{U}^*) = \widehat{L}_Z(\widehat{Z}, \widehat{U}) + [\widehat{L}_{ZZ}(\widehat{Z}, \widehat{U})\{\widehat{Z}^* - \widehat{Z}\}] + [\widehat{L}_{ZU}(\widehat{Z}, \widehat{U})\{\widehat{U}^* - \widehat{U}\}]$$
$$+O(\|\widehat{Z} - \widehat{Z}^*\|^2 + \|\widehat{Z} - \widehat{Z}^*\|\|\widehat{U} - \widehat{U}^*\|)$$

using the linearity of $\widehat{L}(Z, U)$ in U. Note that the terms in square brackets, although involving second-order differentiation, are summed over only one argument and are therefore vectors of length $n(n+1)/2 + m + 1 - t$, the number of variables in Z. This system of equations has a row and a column corresponding to each element of $Z = (x, Y, \omega, \theta)$. Let us *discard* the *rows* corresponding to Y_{11}, and *absorb* the *columns* corresponding to Y_{11} into the O term, which is permissible since $\widehat{Y} = 0$, $\widehat{Y}^*_{11} = O(\|\widehat{x} - x^*\|^2)$. Using the fact that $\widehat{L}_{ZU} = -\widehat{F}_Z$, this gives

$$0 = \widehat{L}_Z(\widehat{Z}, \widehat{U}) + [\widehat{L}_{ZZ}(\widehat{Z}, \widehat{U})\{\widehat{Z}^* - \widehat{Z}\}] - \{\widehat{U}^* - \widehat{U}\} : \widehat{F}_Z(\widehat{Z}) + O(\|\widehat{x} - x^*\|^2) \tag{5.36}$$

system (5.28) are equivalent. Using (4.18)–(4.19), it follows that if $\|\hat{x} - x^*\|$ is sufficiently small, the columns of the linear system (5.32) are also independent. (The fact that the columns of the latter system have more rows than the columns of the former, because of the presence of the additional variables Y_{11}, does not affect the linear independence.) This rank condition provides a constraint qualification guaranteeing the existence and uniqueness of $\hat{U}^*$, satisfying (5.32), i.e.

$$\hat{U}^* : \hat{F}_Z(\hat{Z}^*) = v, \tag{5.34}$$

where v is a vector with one nonzero element, namely 1, in the position corresponding to the variable ω. By definition, $\hat{U}$ satisfies

$$\hat{U} : \hat{F}_Z(\hat{Z}) = v + O(\|\hat{Z} - \hat{Z}^*\|),$$

which has no equations corresponding to Y_{11}. Subtracting this equation from the corresponding equations in (5.34), ignoring the Y_{11} equations in (5.34), and noting that $\hat{F}_Z$ is Lipschitz, gives

$$\{\hat{U} - \hat{U}^*\} : \hat{F}_Z(\hat{Z}) = O(\|\hat{Z} - \hat{Z}^*\|).$$

The independence of the columns of the coefficient matrix defining this system then gives (5.33).

The proof of the final statement of the theorem is as follows. From (5.30),

$$K^*\{K^*\}^T\{\text{vec } U_{11}^*\} = K^* e_1$$

and, from (5.15),

$$\widehat{K}\widehat{K}^T\{\text{vec } \hat{U}_{11}\} = \widehat{K}^T e_1.$$

It follows as a consequence, using (4.19) and the fact that K^* is full rank, that

$$\|\hat{U}_{11} - U_{11}^*\| = O(\|\hat{x} - x^*\|).$$

Combining this equation with (4.19) and (5.30) gives

$$\widehat{K}^T\{\text{vec } \hat{U}_{11}\} = e_1 + O(\|\hat{x} - x^*\|)$$

from which the result follows. ∎

(5.20), $\{\Delta x\}^T W^* \{\Delta x\} = U_{11}^* : M^*$ for all $\{\Delta x\}$, so it follows that W^* is independent of the choice of basis Q_1^*.

4. The null space of K^* is

$$\{v : K^* v = 0\}$$

i.e.

$$\{v = (v_0 \; v_1 \ldots v_m)^T : v_0 I + \sum_{k=1}^{m} v_k \{Q_1^*\}^T \frac{\partial A(x^*)}{\partial x_k} Q_1^* = 0\},$$

which is unchanged if Q_1^* is postmultiplied by an orthogonal matrix.

∎

The previous theorem was concerned only with quantities involving x^* and F^*. In order to prove convergence of Iterations 3 and 4, however, we need to quantify the relationship between $\widehat{U}$ and $\widehat{U}^*$, the latter quantity being the dual matrix associated with the solution of (3.11)–(3.12).

Theorem 5.3 *Suppose K^* has linearly independent rows and that $\widehat{x}$ is sufficiently close to x^*. Consider the nonlinear program (3.11)–(3.12), which has no constraint that $Y_{11} = 0$. A necessary condition for $\widehat{Z}^* = (x^*, \widehat{Y}^*, \lambda_1^*, \Lambda_2^*)$ to solve (3.11)–(3.12) is that there exists an n by n symmetric matrix $\widehat{U}^*$ satisfying*

$$\widehat{L}_Z(\widehat{Z}^*, \widehat{U}^*) = 0, \tag{5.32}$$

i.e. (5.3)–(5.6) hold for $Z = \widehat{Z}^*$, $U = \widehat{U}^*$. Furthermore, $\widehat{U}^*$ is unique. Now assume that the residual of (5.3)–(5.6) with $Z = \widehat{Z}$, $U = \widehat{U}$ is $O(\|\widehat{Z} - \widehat{Z}^*\|)$, as required by Iteration 3. Then

$$\|\widehat{U} - \widehat{U}^*\| = O(\|\widehat{Z} - \widehat{Z}^*\|). \tag{5.33}$$

Furthermore, such a matrix $\widehat{U}$ is obtained by using the block structure (5.11) and solving the least squares problem (5.15).

Proof: From Theorem 5.2, the independence of the rows of K^* and the independence of the columns of the coefficient matrix defining the linear

Proof:

1. The rth singular value of K^* can be written

$$\min_{\|S\|_F=1} \|\{K^*\}^T\{\text{vec } S\}\|,$$

where S is a t by t symmetric matrix. (The quantity (4.12) is zero in the general case that K^* has more columns than rows.) The quantity being minimized is

$$(\{\text{tr } S\}^2 + \sum_{k=1}^{m}\{S : \{Q_1^*\}^T \frac{\partial A(x^*)}{\partial x_k} Q_1^*\}^2\ )^{\frac{1}{2}}.$$

This minimum value is independent of the choice of basis Q_1^*, since any rotation of the basis can be absorbed into S.

2. Let

$$U^* = \begin{bmatrix} U_{11}^* & U_{12}^* \\ \{U_{12}^*\}^T & U_{22}^* \end{bmatrix}.$$

We claim that (5.28) is equivalent to the two conditions (5.29)–(5.30). To see that (5.28) implies (5.29)–(5.30), observe, by analogy with (5.3)–(5.7) and (3.15)–(3.21), that $U^* : F_\Theta^* = 0$ implies the diagonal elements of U_{22}^* are zero, while $U^* : F_{Y_{22}}^*(Z^*) = 0$ and $U^* : F_{Y_{12}}^*(Z^*) = 0$, together with (3.1), imply respectively that the off-diagonal elements of U_{22}^* and all elements of U_{12}^* are zero. The conditions $U^* : F_\omega^* = 1$ and $U^* : F_x^*(Z^*) = 0$ then reduce to (5.30). Conversely, if (5.29)–(5.30) hold, it is easily verified that (5.28) holds. The linear independence of the columns of $\{K^*\}^T$, equivalently the columns of the coefficient matrix of the linear system (5.28), provides a constraint qualification guaranteeing the existence and uniqueness of U^*.

3. Let M^* be defined by (5.25) with $\hat{x}, \hat{\Lambda}, \hat{Q}$ replaced respectively by x^*, Λ^*, Q^*. (This is equivalent to (5.18) in this case since $\lambda_1^* = \cdots = \lambda_t^*$.) When Q_1^* is postmultiplied by a t by t orthogonal matrix P, it has the following effect: the first column of K^* is unchanged and the others are replaced by vec $P^T Q_1^* \frac{\partial A(x^*)}{\partial x_k} Q_1^* P$; the matrix M^* is replaced by $P^T M^* P$; the matrix U_{11}^* is replaced by $P^T U_{11}^* P$. By analogy with

Theorem 5.2

1. *Consider the r by $(m+1)$ matrix K^*, defined by (4.11), where $r = t(t+1)/2$. Then the rth singular value of K^* does not depend on the choice of basis Q_1^*.*

2. *Suppose that the rth singular value of K^* is nonzero, i.e. K^* has linearly independent rows. Consider the nonlinear program (3.23)–(3.25), noting that the latter constraint removes Y_{11} from the variable set. Let*

$$L^*(Z,U) = \omega - U : F^*(Z).$$

A necessary condition for $Z^* = (x^*, 0, \lambda_1^*, \Lambda_2^*)$ to solve (3.23)–(3.25) is that there exists an n by n symmetric matrix U^*, satisfying

$$L_Z^*(Z^*, U^*) = 0. \tag{5.28}$$

Furthermore, U^* is unique, with

$$U^* = \begin{bmatrix} U_{11}^* & 0 \\ 0 & 0 \end{bmatrix}, \tag{5.29}$$

where the t by t block U_{11}^* satisfies

$$\{K^*\}^T \{\text{vec } U_{11}^*\} = e_1. \tag{5.30}$$

3. *Define W^* to be the m by m symmetric matrix with elements*

$$W_{kl}^* = U_{11}^* : G^{*kl}$$

where G^{*kl} is the t by t symmetric matrix with elements

$$G^{*kl} = Q_1^{*T} \frac{\partial^2 A(x^*)}{\partial x_k \partial x_l} Q_1^* + 2\{Q_1^*\}^T \frac{\partial A(x^*)}{\partial x_k} Q_2^* \{\lambda_1^* I - \Lambda_2^*\}^{-1} \{Q_2^*\}^T \frac{\partial A(x^*)}{\partial x_l} Q_1^*.$$

Then W^* is independent of the choice of basis Q_1^*.

4. *The null space of K^* is independent of the choice of basis Q_1^*. Consequently, if N^* is a matrix with orthonormal columns spanning the null space of K^*, the eigenvalues of the reduced Hessian matrix*

$$\{N^*\}^T \begin{bmatrix} 0 & 0 \\ 0 & W^* \end{bmatrix} N^* \tag{5.31}$$

are independent of the choice of bases Q_1^*, N^*. (The matrix in the center of this expression has dimension $m+1$ by $m+1$.)

and

$$\widetilde{W}_{kl} = \widehat{U}_{11} : \widetilde{G}^{kl}. \tag{5.27}$$

The use of $\widetilde{W}$ instead of $\widehat{W}$ does not affect the convergence rate of Iteration 4, but the advantage of the latter formula is that it leads to the following observation, due to M.K.H. Fan[1]:

Theorem 5.1 *Suppose A is an affine function, i.e. $A_{xx} = 0$. Then if $\widehat{U}_{11}$ is positive semi-definite, $\widetilde{W}$ is also positive semi-definite, regardless of the magnitude of $\widehat{x} - x^*$.*

Proof: Since $A_{xx} = 0$, it is clear that, for any choice of Δx, $\widetilde{M}$ is positive semi-definite. Since $\widehat{U}_{11}$ is positive semi-definite, the inner product $\widehat{U}_{11} : \widetilde{M}$ is nonnegative for all Δx, which is equivalent to the condition $\{\Delta x\}^T \widetilde{W} \{\Delta x\} \geq 0$ for all Δx. ∎

Clearly, the same result holds if $[A_{xx}(\widehat{x})\Delta x \Delta x]$ is positive semi-definite for all Δx. Furthermore, if $\widehat{x}$ is close enough to x^*, and $\widetilde{W}$ is positive definite, then $\widehat{W}$ is positive definite. However, even if A is affine, $\widehat{W}$ is not positive semi-definite in general. For example, suppose $n = 3$, $t = 2$, and $\widehat{Q} = I$. The condition that $\widehat{M}$ is positive semi-definite then reduces to the condition $\gamma_{113}\gamma_{223} \geq \gamma_{123}^2$, regardless of A_x. Choosing $\widehat{\Lambda} = \mathrm{Diag}(2, 1, 0)$ gives

$$\gamma_{113} = 1, \quad \gamma_{123} = \gamma_{213} = 1.5, \quad \gamma_{223} = 2.$$

so that $\widehat{M}$ is indefinite. Then $\widehat{U}_{11}$ can be chosen positive semi-definite such that (5.20) is negative. However, substituting $2/(\widehat{\lambda}_1 - \widehat{\lambda}_3)$ for γ_{ijs} results in the matrices $\widetilde{M}$ and $\widetilde{W}$, which are positive semi-definite.

The positive semi-definite condition on $\widehat{U}_{11}$ is a natural one, because, as indicated by the next two theorems, $\widehat{U}_{11}$ is an approximation to the matrix V^* given in (3.4). Specifically, note that equation (5.30) defining U_{11}^* in the following theorem is identical to equation (3.4) defining V^*. There is no condition on the definiteness of U_{11}^*, because in the formulation of the nonlinear program (3.23)–(3.24) we *assumed* that the optimal multiplicity t is known; consequently, indefiniteness of U_{11}^* indicates that t *was chosen incorrectly* and hence that x^* does *not* minimize ϕ.

Again, the case $t = 1$ is instructive: then, since $\widehat{U}_{11} = 1$, $\widehat{G}^{kl}$ is the scalar quantity (1.4) (with $i = 1$), i.e. the second partial derivative of ϕ at $x = \widehat{x}$, and $\widehat{W}$ is the Hessian matrix of ϕ at $x = \widehat{x}$.

Therefore, Iteration 3, with $\widehat{U}$ satisfying (5.11), reduces to:

Iteration 4. Given an initial value $\widehat{x}$:

1. Define $\widehat{\Lambda}$, $\widehat{Q}$ by (1.1)–(1.2).
2. Define $\widehat{U}_{11}$ by any t by t symmetric matrix such that (5.14) holds.
3. Define $\widehat{W}$ by (5.19)–(5.22). Solve the following quadratic program:

$$\min_{\Delta\omega, \Delta x} \quad \Delta\omega + \tfrac{1}{2}\{\Delta x\}^T \widehat{W}\{\Delta x\} \tag{5.23}$$

$$\text{subject to} \qquad \widehat{K}\begin{bmatrix} \Delta\omega \\ \Delta x \end{bmatrix} = \widehat{b} \tag{5.24}$$

   where the latter constraint is defined by (4.6)–(4.7). Set $\overline{x} = \widehat{x} + \Delta x$.
4. Replace $\widehat{x}$ by $\overline{x}$ and go to Step 1.

In the case $t = 1$, we see from (5.16) that (5.23)–(5.24) reduces to the ordinary Newton iteration

$$\min_{\Delta x} \quad [\phi_x(\widehat{x})\Delta x] + \tfrac{1}{2}[\phi_{xx}(\widehat{x})\Delta x \Delta x].$$

Iteration 4 is the method given by [11], with two exceptions: (i) [11] addresses a slightly different problem, namely minimizing $\max(\lambda_1(x), -\lambda_n(x))$, with A assumed to be an affine matrix function; (ii) the method of [11] substitutes the quantities $2/\{\widehat{\lambda}_1 - \widehat{\lambda}_s\}$ for γ_{ijs}, dropping the last term on the right-hand side of (5.19). With this simplification, the corresponding formulas for (5.18), (5.22) can be written conveniently using matrix notation as

$$\widetilde{M} = \widehat{Q}_1^T[A_{xx}(\widehat{x})\Delta x \Delta x]\widehat{Q}_1 + 2\widehat{Q}_1^T[A_x(\widehat{x})\Delta x]\widehat{Q}_2 D^{-1}\widehat{Q}_2^T[A_x(\widehat{x})\Delta x]\widehat{Q}_1 \tag{5.25}$$

with $D = \widehat{\lambda}_1 I - \widehat{\Lambda}_2$,

$$\widetilde{G}^{kl} = \widehat{Q}_1^T \frac{\partial^2 A(\widehat{x})}{\partial x_k \partial x_l}\widehat{Q}_1 + 2\widehat{Q}_1^T \frac{\partial A(\widehat{x})}{\partial x_k}\widehat{Q}_2 D^{-1}\widehat{Q}_2^T \frac{\partial A(\widehat{x})}{\partial x_l}\widehat{Q}_1 \tag{5.26}$$

But since ΔY must satisfy the constraint (5.9), whose 1,2 block is (4.8), we see that

$$[\hat{F}_{YY}(\hat{Z})\Delta Y\Delta Y]_{11} = -[\hat{F}_{xY}(\hat{Z})\Delta x\Delta Y]_{11}. \tag{5.17}$$

We therefore have

$$\begin{aligned}[\hat{F}_{ZZ}(\hat{Z})\Delta Z\Delta Z]_{11} &= [\hat{F}_{xx}(\hat{Z})\Delta x\Delta x]_{11} + [\hat{F}_{xY}(\hat{Z})\Delta x\Delta Y]_{11} \\ &\quad +[\hat{F}_{Yx}(\hat{Z})\Delta Y\Delta x]_{11} + [\hat{F}_{YY}(\hat{Z})\Delta x\Delta Y]_{11} \\ &= -\hat{Q}_1^T[A_{xx}(\hat{x})\Delta x\Delta x]\hat{Q}_1 + \{\Delta Y\}_{12}\hat{Q}_2^T[A_x(\hat{x})\Delta x]\hat{Q}_1 \\ &\quad +\hat{Q}_1^T[A_x(\hat{x})\Delta x]\hat{Q}_2\{\Delta Y\}_{12}^T.\end{aligned}$$

Let us denote the right-hand side of this equation by $-\widehat{M}$; then we see that, under the constraints (5.9)–(5.10),

$$[\hat{L}_{ZZ}(\hat{Z},\hat{U})\Delta Z\Delta Z] = \hat{U}_{11} : \widehat{M}.$$

Using (4.8) we see that the elements of the $t \times t$ matrix $\widehat{M}$ are given by

$$\widehat{M}_{ij} = \hat{q}_i^T[A_{xx}(\hat{x})\Delta x\Delta x]\hat{q}_j + \sum_{s=t+1}^{n} \gamma_{ijs}\hat{q}_i^T[A_x\Delta x]\hat{q}_s \ \hat{q}_j^T[A_x\Delta x]\hat{q}_s \tag{5.18}$$

where $1 \le i \le t$, $1 \le j \le t$ and

$$\gamma_{ijs} = \frac{1}{\hat{\lambda}_i - \hat{\lambda}_s} + \frac{1}{\hat{\lambda}_j - \hat{\lambda}_s} = \frac{2}{\hat{\lambda}_1 - \hat{\lambda}_s} + O(\|\hat{x} - x^*\|). \tag{5.19}$$

Writing out the double sums in the square brackets explicitly we see that, under the constraints (5.9)–(5.10),

$$[\hat{L}_{ZZ}(\hat{Z},\hat{U})\Delta Z\Delta Z] = \hat{U}_{11} : \widehat{M} = \{\Delta x\}^T\widehat{W}\{\Delta x\} \tag{5.20}$$

where $\widehat{W}$ is an m by m symmetric matrix whose k,l element satisfies

$$\widehat{W}_{kl} = \hat{U}_{11} : \hat{G}^{kl} \tag{5.21}$$

with $\hat{G}^{kl}$ defined to be the t by t symmetric matrix with elements

$$\{\hat{G}^{kl}\}_{ij} = \hat{q}_i^T\frac{\partial^2 A(\hat{x})}{\partial x_k \partial x_l}\hat{q}_j + \sum_{s=t+1}^{n} \gamma_{ijs}\hat{q}_i^T\frac{\partial A(\hat{x})}{\partial x_k}\hat{q}_s \ \hat{q}_j^T\frac{\partial A(\hat{x})}{\partial x_l}\hat{q}_s. \tag{5.22}$$

As we shall see in Theorem 5.3 below, this can be achieved by solving the least squares problem

$$\min_{\widehat{U}_{11}} \|\widehat{K}^T\{\text{vec } \widehat{U}_{11}\} - e_1\|. \tag{5.15}$$

The constraints (5.9)–(5.10) are identical to the condition in Step 2 of Iteration 1, the only difference being that the system of linear equations is underdetermined rather than square. The same argument given following Iteration 1 therefore shows that (5.9)–(5.10) is equivalent to the constraint (4.5) on Δx, $\Delta\omega$ together with (4.8),(4.10) defining $\{\Delta Y\}_{12}$, $\{\Delta Y\}_{22}$.

It is instructive to consider the special case $t = 1$ at this point: in this case the max eigenvalue function $\phi(x)$ is differentiable at x^*. Then $\widehat{Q}_1$ consists of a single column $\widehat{q}_1$, $\widehat{U}_{11}$ is a scalar which can be taken to be the number 1, (5.13) states that the gradient of ϕ at $x = \widehat{x}$ is $O(\|\widehat{x} - x^*\|)$, and the constraint (4.5) states that

$$\Delta\omega = [\phi_x \Delta x]. \tag{5.16}$$

Now let us consider the quadratic objective function (5.8). The linear term may be replaced by $\Delta\omega$, since the rest of this term is fixed by the constraint (5.9). To evaluate the quadratic term in (5.8), we need to calculate the second derivatives of $\widehat{F}$. Clearly, all terms involving ω or Θ are zero. Differentiating (3.13)–(3.14) we obtain

$$\begin{aligned}
[\widehat{F}_{xx}(\widehat{Z})\Delta x\Delta x] &= -\widehat{Q}^T[A_{xx}(\widehat{x})\Delta x\Delta x]\widehat{Q};\\
[\widehat{F}_{xY}(\widehat{Z})\Delta x\Delta Y] &= [\widehat{F}_{Yx}(\widehat{Z})\Delta Y\Delta x]\\
&= \{\Delta Y\}\widehat{Q}^T[A_x(\widehat{x})\Delta x]\widehat{Q} - \widehat{Q}^T[A_x(\widehat{x})\Delta x]\widehat{Q}\{\Delta Y\};\\
[\widehat{F}_{YY}(\widehat{Z})\Delta Y\Delta Y] &= \Delta Y\{\widehat{\Lambda}\{\Delta Y\} - \{\Delta Y\}\widehat{\Lambda}\} - \{\widehat{\Lambda}\{\Delta Y\} - \{\Delta Y\}\widehat{\Lambda}\}\Delta Y.
\end{aligned}$$

Since $\widehat{U}$ satisfies (5.11), we need only the 1,1 block of each of these terms. Using (5.10) and (3.17), we obtain

$$\begin{aligned}
[\widehat{F}_{xx}(\widehat{Z})\Delta x\Delta x]_{11} &= -\widehat{Q}_1^T[A_{xx}(\widehat{x})\Delta x\Delta x]\widehat{Q}_1;\\
[\widehat{F}_{xY}(\widehat{Z})\Delta x\Delta Y]_{11} &= \{\Delta Y\}_{12}\widehat{Q}_2^T[A_x(\widehat{x})\Delta x]\widehat{Q}_1 + \widehat{Q}_1^T[A_x(\widehat{x})\Delta x]\widehat{Q}_2\{\Delta Y\}_{12}^T;\\
[\widehat{F}_{YY}(\widehat{Z})\Delta Y\Delta Y]_{11} &= \{\Delta Y\}_{12}\{-\widehat{\Lambda}_2\{\Delta Y\}_{12}^T + \{\Delta Y\}_{12}^T\widehat{\Lambda}_1\} +\\
&\quad \{\widehat{\Lambda}_1\{\Delta Y\}_{12} - \{\Delta Y\}_{12}\widehat{\Lambda}_2\}\{\Delta Y\}_{12}^T.
\end{aligned}$$

Iteration 3. Given an initial value $\widehat{x}$:

1. Define $\widehat{\Lambda}$, $\widehat{Q}$ by (1.1)–(1.2), and $\widehat{F}$ by (3.9). Let $\widehat{Z} = \{\widehat{x}, 0, \widehat{\lambda}_1, \widehat{\Lambda}_2\}$.

2. Define $\widehat{U}$ to be any $n \times n$ symmetric matrix such that the norm of the residual of equations (5.3),(5.7),(5.5),(5.6), with $Z = \widehat{Z}$, $U = \widehat{U}$, is $O(\|\widehat{Z} - \widehat{Z}^*\|)$.

3. Solve the quadratic program

$$\min_{\Delta Z} \quad [\widehat{L}_Z(\widehat{Z}, \widehat{U})\Delta Z] + \tfrac{1}{2}[\widehat{L}_{ZZ}(\widehat{Z}, \widehat{U})\Delta Z \Delta Z] \tag{5.8}$$

$$\text{subject to} \qquad [\widehat{F}_Z(\widehat{Z})\Delta Z] = -\widehat{F}(\widehat{Z}) \tag{5.9}$$

   with the restriction also that

$$\{\Delta Y\}_{11} = 0. \tag{5.10}$$

   Set $\overline{Z} = \widehat{Z} + \Delta Z$.

4. Replace $\widehat{x}$ by $\overline{x}$, the x component of $\overline{Z}$. Go to Step 1.

Like Iteration 1, Iteration 3 can be substantially simplified using the structure of the problem. We begin with a closer look at the dual matrix. Suppose we choose

$$\widehat{U} = \begin{bmatrix} \widehat{U}_{11} & 0 \\ 0 & 0 \end{bmatrix}. \tag{5.11}$$

and consider (5.3)–(5.6) with $Z = \widehat{Z}$, $U = \widehat{U}$. We see then that, for $U = \widehat{U}$, (3.16) implies (5.6) and (3.21) implies (5.4). In order to satisfy the condition in Step 2, then, we see from (3.15) and (3.20) that we need only ensure that

$$\text{tr } \widehat{U}_{11} = 1 + O(\|\widehat{x} - x^*\|) \tag{5.12}$$

and

$$\widehat{U}_{11} : \widehat{Q}_1^T \frac{\partial A(\widehat{x})}{\partial x_k} \widehat{Q}_1 = O(\|\widehat{x} - x^*\|), \quad 1 \le k \le m. \tag{5.13}$$

This is a system of $m + 1$ equations in $\frac{t(t+1)}{2}$ unknowns, which can also be written

$$\widehat{K}^T \{\text{vec } \widehat{U}_{11}\} = e_1 + O(\|\widehat{x} - x^*\|). \tag{5.14}$$

where U is an $n \times n$ symmetric matrix of Lagrange multipliers corresponding to the $n \times n$ symmetric matrix constraint (3.12). The matrix U is called the *dual matrix* since its components are dual variables. The Frobenius inner product $A : B$ was defined at the end of Section 2. Assuming a full rank condition to be discussed in detail later, the first-order necessary conditions for Z to minimize (3.11) subject to (3.12) are that, in addition to the satisfaction of (3.12) by Z, there exists U satisfying

$$\widehat{L}_Z(Z, U) = 0, \tag{5.2}$$

i.e.

$$U : \widehat{F}_x(Z) = 0, \tag{5.3}$$

$$U : \widehat{F}_Y(Z) = 0, \tag{5.4}$$

$$U : \widehat{F}_\omega = 1, \tag{5.5}$$

and

$$U : \widehat{F}_\Theta = 0. \tag{5.6}$$

Here (5.3), for example, is understood to mean $U : [\widehat{F}_x(Z)\Delta x] = 0$ for all Δx, i.e. $U : \frac{\partial \widehat{F}(Z)}{\partial x_k} = 0$, $1 \leq k \leq m$. A pair Z, U which satisfies conditions (5.3)–(5.6) is denoted $\widehat{Z}^*, \widehat{U}^*$.

In the following Newton iteration we shall, as in the previous section, impose the additional condition that $\{\Delta Y\}_{11} = 0$, and we shall therefore also *relax* the corresponding dual condition $U : \widehat{F}_{\{Y_{11}\}}(Z) = 0$, replacing (5.4) by

$$U : \widehat{F}_{\{Y_{12}\}}(Z) = 0, \qquad U : \widehat{F}_{\{Y_{22}\}}(Z) = 0. \tag{5.7}$$

Each step of the iteration requires a dual matrix *estimate* $\widehat{U}$, which is necessary to define the Lagrangian function. It is important to note that a dual matrix estimate from the *previous* step of the iteration *cannot* be used, since the function $\widehat{F}$ changes from one iteration to the next, with the basis $\widehat{Q}$, which defines $\widehat{F}$, not converging in general.

all of the derivatives being evaluated at $\widehat{Z}$, the appearance of $O(\|\widehat{x} - x^*\|^2)$ instead of $O(\|\widehat{Z} - \widehat{Z}^*\|^2)$ on the right-hand side being justified by (3.27). By Theorem 3.1, the $\widehat{F}_{\{Y_{11}\}}$ term on the left-hand side can be absorbed into the right-hand side, reducing (4.16) to a linear system of $\frac{n(n+1)}{2}$ equations in $\frac{n(n+1)}{2}$ variables. By precisely the argument which showed the equivalence of (4.1)–(4.2) with (4.5),(4.8),(4.10), this system can be reduced to $\frac{t(t+1)}{2}$ equations in $\frac{t(t+1)}{2}$ unknowns, namely

$$\widehat{K}\begin{bmatrix} \widehat{\lambda}_1 + \Delta\omega - \lambda_1^* \\ \overline{x} - x^* \end{bmatrix} = O(\|\widehat{x} - x^*\|^2). \tag{4.17}$$

The proof is then complete if we can assert that the norm of the inverse of $\widehat{K}$ is bounded for $\widehat{x}$ in a neighborhood of x^*. Theorem 3.1 shows that there is an orthonormal basis of eigenvectors for $A(x^*)$, namely $Q^* = \widehat{Q}e^{\widehat{Y}^*}$, for which

$$\|\widehat{Q} - Q^*\| = \|\widehat{Q}^T(\widehat{Q} - Q^*)\| = \|I - e^{\widehat{Y}^*}\| = O(\|\widehat{Y}^*\|) = O(\|\widehat{x} - x^*\|). \tag{4.18}$$

Using this choice of Q^* in (4.11), we have

$$\|\widehat{K} - K^*\| = O(\|\widehat{x} - x^*\|). \tag{4.19}$$

Since K^* is nonsingular by assumption, and this nonsingularity is independent of the basis choice, the boundedness of the inverse of $\widehat{K}$ follows from the standard Banach lemma. ∎

5 The General Case

In this section we assume that $\frac{t(t+1)}{2} \leq m + 1$. The von Neumann-Wigner argument discussed earlier shows that the opposite inequality can hold only nongenerically. Equality can be expected to hold only occasionally since relatively few of the integers have the form $\frac{t(t+1)}{2}$. In the general case, the constraints (3.12) are not enough to define x^* locally, so minimization of (3.11) must also be considered.

Define the Lagrangian function for (3.11)–(3.12) by

$$\widehat{L}(Z, U) = \omega - U : \widehat{F}(Z) \tag{5.1}$$

(see the discussion at the end of Section 2). This quantity is not changed if Q_1^* is postmultiplied by an orthogonal matrix. ∎

Using this result, we can speak unambiguously about whether or not K^* is singular. The convergence result may now be stated.

Theorem 4.2 *Suppose K^* is nonsingular. Then there exist constants ϵ and C such that, if $\|\widehat{x} - x^*\| \leq \epsilon$, then*

$$\|\overline{x} - x^*\| \leq C\|\widehat{x} - x^*\|^2.$$

Consequently, Iteration 1, equivalently Iteration 2, generates points $\widehat{x}$ which converge quadratically to the solution x^*.

Proof: That Iterations 1 and 2 generate the same point $\widehat{x}$ follows from the equivalence of (4.1)–(4.2) with (4.5), (4.8),(4.10). Expanding $\widehat{F}$ in a Taylor series about $\widehat{Z}$, using the point $\widehat{Z}^*$ whose existence is guaranteed by Theorem 3.1, gives

$$0 = \widehat{F}(\widehat{Z}^*) = \widehat{F}(\widehat{Z}) + [\widehat{F}_Z(\widehat{Z})\{\widehat{Z}^* - \widehat{Z}\}] + O(\|\widehat{Z} - \widehat{Z}^*\|^2). \tag{4.13}$$

By definition of Iteration 1, we also have

$$0 = \widehat{F}(\widehat{Z}) + [\widehat{F}_Z(\widehat{Z})\{\overline{Z} - \widehat{Z}\}], \tag{4.14}$$

noting that the Y_{11} component of $\overline{Z}$ is zero. The difference of these two equations gives

$$[\widehat{F}_Z(\widehat{Z})\{\overline{Z} - \widehat{Z}^*\}] = O(\|\widehat{Z} - \widehat{Z}^*\|^2). \tag{4.15}$$

Some comments here will be helpful: as usual, the proof of convergence of Newton's method involves three points: the current iterate, the new iterate, and the solution point. Here, these are respectively $\widehat{Z}$, $\overline{Z}$ and $\widehat{Z}^*$, the subtlety being that $\widehat{Z}^*$ is the solution to $\widehat{F}(Z) = 0$, an equation whose definition depends on $\widehat{Z}$. Equation (4.15) states that

$$[\widehat{F}_x\{\overline{x} - x^*\}] +$$

$$[\widehat{F}_{\{Y_{11}\}}\{-\widehat{Y}_{11}^*\}] + [\widehat{F}_{\{Y_{12}\}}\{\{\Delta Y\}_{12} - \widehat{Y}_{12}^*\}] + [\widehat{F}_{\{Y_{22}\}}\{\{\Delta Y\}_{22} - \widehat{Y}_{22}^*\}] +$$
$$[\widehat{F}_\omega\{\widehat{\lambda}_1 + \Delta\omega - \lambda_1^*\}] + [\widehat{F}_\Theta\{\widehat{\Lambda}_2 + \Delta\Theta - \Lambda_2^*\}] = O(\|\widehat{x} - x^*\|^2), \tag{4.16}$$

The off-diagonal equations of this symmetric system can be solved for $\{\Delta Y\}_{22}$ in a manner similar to equation (4.9), while the diagonal equations, which vanish in the last two terms, can be solved for $\Delta\Theta$.

In fact, though, we see that each step of Iteration 1 actually requires solving *only* one linear system for $\Delta\omega$ and Δx, namely (4.5), a system of $\frac{t(t+1)}{2}$ linear equations in $m+1$ variables and therefore square by assumption. The variables ΔY and $\Delta\Theta$ are *not required* to continue with the next iteration; their only purpose is their use in the problem formulation and convergence analysis. Iteration 1 is therefore equivalent to:

Iteration 2. Given an initial value $\widehat{x}$:

1. Define $\widehat{\Lambda}$, $\widehat{Q}$ by (1.1)–(1.2).
2. Solve the linear system $\widehat{K}\begin{bmatrix} \Delta\omega \\ \Delta x \end{bmatrix} = \widehat{b}$, defined in (4.6)–(4.7), for $\Delta\omega$, Δx. Set $\overline{x} = \widehat{x} + \Delta x$.
3. Replace $\widehat{x}$ by $\overline{x}$, and go to Step 1.

Let us now analyze the rate of convergence of Iteration 1, equivalently Iteration 2. We first need:

Theorem 4.1 *Define*

$$K^* = [\text{vec } I \quad -\text{vec } (Q_1^{*T}\frac{\partial A(x^*)}{\partial x_1}Q_1^*) \ \ldots \ -\text{vec } (Q_1^{*T}\frac{\partial A(x^*)}{\partial x_m}Q_1^*)]. \quad (4.11)$$

Then the smallest singular value of K^* is independent of the choice of basis Q_1^*.

Proof: The freedom in Q_1^* is that it may be postmultiplied by any t by t orthogonal matrix. The smallest singular value of K^* is, by definition,

$$\min_{\Delta\omega^2+\|\Delta x\|^2=1} \|K^*\begin{bmatrix} \Delta\omega \\ \Delta x \end{bmatrix}\|. \quad (4.12)$$

The vector norm being minimized is in fact

$$\|\Delta\omega\ I - \{Q_1^*\}^T[A_x(x^*)\Delta x]Q_1^*\|_F$$

situation is not unusual; see [5,15]. The linear system (4.1) is equivalent to

$$[\widehat{F}_x(\widehat{Z})\Delta x] + [\widehat{F}_Y(\widehat{Z})\Delta Y] + [\widehat{F}_\omega(\widehat{Z})\Delta\omega] + [\widehat{F}_\Theta(\widehat{Z})\Delta\Theta] = -\widehat{F}(\widehat{Z}). \quad (4.3)$$

Because of the assumption that $\frac{t(t+1)}{2} = m+1$, together with the fact that Y_{11} is constrained to be zero, this is a system of $\frac{n(n+1)}{2}$ equations in the same number of variables. Examining (3.15)–(3.21), we see that it separates very conveniently. Imposing the condition $\{\Delta Y\}_{11} = 0$, the 1,1 block of (4.3) reduces to the t by t symmetric matrix equation

$$\Delta\omega\ I - \widehat{Q}_1^T[A_x(\widehat{x})\Delta x]\widehat{Q}_1 = \widehat{\Lambda}_1 - \widehat{\lambda}_1 I. \quad (4.4)$$

Let us denote this system of linear equations by

$$\widehat{K}\begin{bmatrix} \Delta\omega \\ \Delta x \end{bmatrix} = \widehat{b} \quad (4.5)$$

where

$$\widehat{K} = [\text{vec } I \quad -\text{vec } (\widehat{Q}_1^T \frac{\partial A(\widehat{x})}{\partial x_1}\widehat{Q}_1) \ \ldots \ -\text{vec } (\widehat{Q}_1^T \frac{\partial A(\widehat{x})}{\partial x_m}\widehat{Q}_1)] \quad (4.6)$$

and

$$\widehat{b} = \text{vec } (\widehat{\Lambda}_1 - \widehat{\lambda}_1 I). \quad (4.7)$$

Note that $\widehat{K}$ has dimension $t(t+1)/2$ by $m+1$, i.e. it is square under the assumptions of this section. (The operator "vec" was defined at the end of Section 2.)

The 1,2 block of (4.3) is the t by $n-t$ matrix equation

$$-\widehat{Q}_1^T[A_x(\widehat{x})\Delta x]\widehat{Q}_2 - \widehat{\Lambda}_1\{\Delta Y\}_{12} + \{\Delta Y\}_{12}\widehat{\Lambda}_2 = 0 \quad (4.8)$$

which can be solved for $\{\Delta Y\}_{12}$ in terms of Δx by

$$\Delta y_{ij} = \frac{\widehat{q}_i^T[A_x(\widehat{x})\Delta x]\widehat{q}_j}{\widehat{\lambda}_j - \widehat{\lambda}_i}, \quad (4.9)$$

for $1 \le i \le t$, $t < j \le n$; the denominator is bounded away from zero for $\widehat{x}$ in a small enough neighborhood of x^*. The 2,1 block of (4.3) contains the same information as the 1,2 block. The 2,2 block of (4.3) is

$$\Delta\Theta - \widehat{Q}_2^T[A_x(\widehat{x})\Delta x]\widehat{Q}_2 - \widehat{\Lambda}_2\{\Delta Y\}_{22} + \{\Delta Y\}_{22}\widehat{\Lambda}_2 = 0. \quad (4.10)$$

from (3.11)–(3.12) makes (3.12) infeasible in general. Ideally, we would like to work with the function F^*, but Q^* is not known. We shall see that the solution to these difficulties is to work with a different function $\widehat{F}$ at each step of the iteration, removing Y_{11} from each linearization step, but including Y_{11} in the convergence analysis of this procedure.

An immediate consequence of Theorem 3.1 which we shall need later is

$$\|\widehat{Z} - \widehat{Z}^*\| = O(\|\widehat{x} - x^*\|), \tag{3.27}$$

using (3.18) and the Lipschitz continuity of the eigenvalues.

The rest of the paper is organized as follows. In the next section, we analyze the special case $\frac{t(t+1)}{2} = m + 1$, when the dimension of the variable space matches the number of conditions imposed by the multiple eigenvalue, and hence quadratic convergence to a local solution of (1.5) can be achieved by a method which only uses first derivative information. In the subsequent section, we consider the general case, where second derivative information is necessary.

4 A Special Case

In this section we assume $\frac{t(t+1)}{2} = m + 1$, where t, as before, is the multiplicity of λ_1^*. Consider the following iteration.

Iteration 1. Given an initial value $\widehat{x}$:

1. Define $\widehat{\Lambda}$, $\widehat{Q}$ by (1.1)–(1.2), and $\widehat{F}$ by (3.9). Let $\widehat{Z} = \{\widehat{x}, 0, \widehat{\lambda}_1, \widehat{\Lambda}_2\}$.

2. Solve the n by n symmetric matrix equation

$$[\widehat{F}_Z(\widehat{Z})\Delta Z] = -\widehat{F}(\widehat{Z}) \tag{4.1}$$

   for ΔZ, imposing also the condition

$$\{\Delta Y\}_{11} = 0. \tag{4.2}$$

   Set $\overline{Z} = \widehat{Z} + \Delta Z$.

3. Replace $\widehat{x}$ by $\overline{x}$, the x component of $\overline{Z}$. Go to Step 1.

Iteration 1 consists of a *Newton iteration applied to a varying function*, since the function which is differentiated, $\widehat{F}$, changes at each step. Such a

called B there is not bounded. The statement should instead have been made that the methods essentially result from applying Newton's method to the function (3.12) (in the inverse eigenvalue context ω and Θ are fixed); in other words, the $t \times t$ block of equations corresponding to the multiple eigenvalue cannot simply be analyzed separately from the other equations. However, although this motivational attempt was misguided, the methods themselves are correct as given in [4] and [11], and the convergence analysis in [4] is also correct.

But now a second key point must be emphasized. Although the Y_{11} variables are redundant in (3.23)–(3.24), they are *not* redundant in (3.11)–(3.12) if $\widehat{x} \neq x^*$; on the contrary, the *freedom in* Y_{11} *is necessary* to ensure that a feasible solution to $\widehat{F}(Z) = 0$ exists in general. Clearly, the closer $\widehat{x}$ is to x^*, the closer the Y_{11} variables come to being redundant; this observation is quantified by the following theorem, which follows directly from [4], Corollary 3.1 and subsequent remarks.

Theorem 3.1 *There exist* $\epsilon > 0$, $C < \infty$ *such that, if* $\|\widehat{x} - x^*\| \leq \epsilon$, *then* $\widehat{F}(Z) = 0$ *has a solution* $\widehat{Z}^* = \{x^*, \widehat{Y}^*, \lambda_1^*, \Lambda_2^*\}$ *with*

$$\|\widehat{Y}^*\| \leq C\|\widehat{x} - x^*\|$$

and with the leading t *by* t *block of* $\widehat{Y}^*$ *satisfying*

$$\|\widehat{Y}_{11}^*\| \leq C\|\widehat{x} - x^*\|^2.$$

Here $\widehat{Y}^*$ *and* $\widehat{Z}^*$ *are so denoted because, unlike* x^*, *they depend on the choice of function* $\widehat{F}$.

Roughly speaking, the Y variables describe the rotation of the eigenvectors $\widehat{q}_i$ needed to transform them to eigenvectors of $A(x^*)$, while Y_{11} describes the rotation of the first t of these eigenvectors within the t-dimensional space they span. The rotation of the latter kind becomes relatively unimportant, as $\widehat{x} \to x^*$, because of the nonuniqueness of the eigenvectors of $A(x^*)$.

Straightforward application of Newton's method to solve (3.11)–(3.12) is not satisfactory, since inclusion of the Y_{11} variables, which are redundant in the limit, prevents rapid convergence. On the other hand, removing Y_{11}

Thus, $\widehat{F}$ and F^* coincide if $\widehat{x} = x^*$ and the same basis $\widehat{Q} = Q^*$ is used in both definitions. Since Λ_1^* is a multiple of the identity matrix, it is clear, by analogy with (3.21), that *all contributions from* Y_{11} *vanish* from the derivatives of F^*. Therefore, in the nonlinear program

$$\min_{x,Y,\omega,\Theta} \quad \omega \tag{3.23}$$

$$\text{subject to} \quad F^*(x, Y, \omega, \Theta) = 0 \tag{3.24}$$

neither the minimization objective nor the constraint Jacobian at the solution x^* depends on Y_{11}, i.e. the rows of the gradients of the objective and constraint functions which correspond to the elements of Y_{11} are all zero. Consequently, these variables have no effect on the Lagrange multiplier system at x^* and could be eliminated by setting

$$Y_{11} = 0. \tag{3.25}$$

Removing Y_{11} changes (3.24) to a system of $\frac{n(n+1)}{2}$ equations in $\frac{n(n+1)}{2} + m + 1 - \frac{t(t+1)}{2}$ unknowns.

Thus, we recover the von Neumann–Wigner dimension count mentioned above; imposing the multiple eigenvalue equation (3.12) represents $\frac{t(t+1)}{2}$ generic degrees of restriction on a parameter space of dimension $m+1$ (the m elements of x and the common maximum value ω).

The discussion just given is very closely related to that in [4]. Indeed, the function F^* was given in Theorem 3.1, p.654, in explaining when an inverse eigenvalue problem with multiple eigenvalues is well-posed. The observation that the partial derivatives of F^* with respect to Y_{11} are zero was not explicitly made, although the subsequent Lemma 3.1 states a closely related fact. Also, the statement was made, both in [4, p.650] and in [11, p.260], that the quadratically convergent methods given in those papers essentially result from applying Newton's method to the system of $\frac{t(t+1)}{2}$ nonlinear equations

$$Q_1(x)^T A(x) Q_1(x) = \omega I \tag{3.26}$$

where $Q_1(x)$ is a locally (near $\widehat{x} \neq x^*$) smoothly varying basis of eigenvectors of $A(x)$ corresponding to the largest t eigenvalues. It was pointed out by [19] that this is clearly incorrect, since all off-diagonal equations are identically zero. The fallacy in the remarks in [4], p.650, is that the matrix

$$[\widehat{F}_Y \Delta Y] = -B - B^T, \quad \text{where} \tag{3.14}$$

$$B = \{-\Delta Y + \tfrac{1}{2}\{\Delta Y\}Y + \tfrac{1}{2}Y\{\Delta Y\} + O(Y^2)\}\widehat{Q}^T A(x)\widehat{Q}\{I + Y + O(Y^2)\};$$

$$[\widehat{F}_\omega \Delta\omega] = \begin{bmatrix} \Delta\omega\ I & 0 \\ 0 & 0 \end{bmatrix}; \tag{3.15}$$

$$[\widehat{F}_\Theta \Delta\Theta] = \begin{bmatrix} 0 & 0 \\ 0 & \Delta\Theta \end{bmatrix}. \tag{3.16}$$

Here $\Delta x, \Delta Y, \Delta\omega, \Delta\Theta$ are variables with the same dimensions as x, Y, ω, Θ, respectively; for example ΔY, like Y, is an n by n skew-symmetric matrix, with

$$\Delta Y = \begin{bmatrix} \{\Delta Y\}_{11} & \{\Delta Y\}_{12} \\ -\{\Delta Y\}_{12}^T & \{\Delta Y\}_{22} \end{bmatrix}, \tag{3.17}$$

where ΔY_{11} and ΔY_{22} are skew-symmetric (but ΔY_{12} is not).

It will be convenient to denote the variables $\{x, Y, \omega, \Theta\}$ collectively by a single variable Z, which lies in a space of dimension $\frac{n(n+1)}{2} + m + 1 - t$. Likewise, ΔZ denotes $\{\Delta x, \Delta Y, \Delta\omega, \Delta\Theta\}$.

Now let us evaluate $\widehat{F}$ and its derivatives $\widehat{F}_x$, $\widehat{F}_Y$ at the point

$$\widehat{Z} = \{\widehat{x}, \widehat{Y}, \widehat{\lambda}_1, \widehat{\Lambda}_2\}, \tag{3.18}$$

where

$$\widehat{Y} = 0$$

the latter equation being essential to keep the formulas simple. The other derivatives $\widehat{F}_\omega$ and $\widehat{F}_\Theta$ are constant. We have

$$\widehat{F}(\widehat{Z}) = \begin{bmatrix} \widehat{\lambda}_1 I - \widehat{\Lambda}_1 & 0 \\ 0 & 0 \end{bmatrix}; \tag{3.19}$$

$$[\widehat{F}_x(\widehat{Z})\Delta x] = -\widehat{Q}^T[A_x(\widehat{x})\Delta x]\widehat{Q}; \tag{3.20}$$

$$[\widehat{F}_Y(\widehat{Z})\Delta Y] = -\widehat{\Lambda}\{\Delta Y\} + \{\Delta Y\}\widehat{\Lambda} = \tag{3.21}$$

$$\begin{bmatrix} -\widehat{\Lambda}_1\{\Delta Y\}_{11} + \{\Delta Y\}_{11}\widehat{\Lambda}_1 & -\widehat{\Lambda}_1\{\Delta Y\}_{12} + \{\Delta Y\}_{12}\widehat{\Lambda}_2 \\ \widehat{\Lambda}_2\{\Delta Y\}_{12}^T - \{\Delta Y\}_{12}^T\widehat{\Lambda}_1 & -\widehat{\Lambda}_2\{\Delta Y\}_{22} + \{\Delta Y\}_{22}\widehat{\Lambda}_2 \end{bmatrix}.$$

Now comes a key observation. Define

$$F^*(x, Y, \omega, \Theta) = \begin{bmatrix} \omega I & 0 \\ 0 & \Theta \end{bmatrix} - e^{-Y}(Q^*)^T A(x) Q^* e^Y. \tag{3.22}$$

the context, it is clear that I is used to mean the identity matrix of order t; subsequent block matrices will have dimensions conforming with those of $\widehat{F}$. We shall find it useful to write

$$Y = \begin{bmatrix} Y_{11} & Y_{12} \\ -{Y_{12}}^T & Y_{22} \end{bmatrix}, \tag{3.10}$$

where Y_{11} and Y_{22} are skew-symmetric but Y_{12} is not. Note that the definition of $\widehat{F}$ depends on $\widehat{x}$ through $\widehat{Q}$.

Consider the nonlinear program

$$\min_{x,Y,\omega,\Theta} \qquad \omega \tag{3.11}$$

$$\text{subject to} \quad \widehat{F}(x,Y,\omega,\Theta) = 0. \tag{3.12}$$

It is clear that if $\{x,Y,\omega,\Theta\}$ solves (3.12), then $\{x,\omega\}$ satisfies the constraints (3.6), with $A(x)$ having eigenvalues $\omega,\ldots,\omega$, $\theta_1,\ldots\theta_{n-t}$, and eigenvectors given by the columns of $\widehat{Q}e^Y$. Conversely, if x,ω satisfy (3.6), then, regardless of $\widehat{Q}$, (3.12) has a solution $\{x,Y,\omega,\Theta\}$, with $\theta_i = \lambda_{t+i}(x)$ and $e^Y = \widehat{Q}^T Q$, where Q is an orthogonal matrix of eigenvectors for $A(x)$. Consequently, given that (3.1) holds, formulation (1.5), formulation (3.5)–(3.6) and formulation (3.11)–(3.12) are all equivalent, regardless of the choice of $\widehat{x}$.

Comparing (3.11)–(3.12) with (3.5)–(3.6), we see that we have introduced an additional $\frac{n(n+1)}{2} - t$ equations and the same number of additional variables (since Y is skew-symmetric). Thus, (3.12) consists of $\frac{n(n+1)}{2}$ equations in $\frac{n(n+1)}{2} + m + 1 - t$ variables. The important point is that $\widehat{F}$ is (Fréchet) differentiable. Consequently, if its derivative has full row rank, $\frac{n(n+1)}{2}$, the standard Lagrange multiplier rule may be applied, e.g. [3], stating that a necessary condition for $\{x,Y,\omega,\Theta\}$ to be a solution of the nonlinear program (3.11)–(3.12) is that the gradient of the objective function in (3.11) is a linear combination of the gradients of the $\frac{n(n+1)}{2}$ component functions making up $\widehat{F}$.

Let us calculate the derivatives of $\widehat{F}$. The appearance of the matrix exponential function in the definition makes this an easy task. We obtain

$$[\widehat{F}_x \Delta x] = -e^{-Y}\widehat{Q}^T[A_x(x)\Delta x]\widehat{Q}e^Y; \tag{3.13}$$

V^*, are satisfied. See [12] for discussion of the case where all optimality conditions except the positive semi-definite condition are satisfied.

Assuming, then, that the optimal value of t is known, solving (1.5) is equivalent to

$$\min_{x,\omega} \quad \omega \tag{3.5}$$

$$\text{subject to} \quad \omega = \lambda_i(x), \ i = 1, \ldots, t. \tag{3.6}$$

where $x \in \Re^m$ and ω is a real scalar. This is apparently a nonlinear program with $m+1$ variables and t constraints, but since the constraints are not differentiable, we cannot apply standard Lagrange multiplier techniques. However, since the constraints now have the same form as an inverse eigenvalue problem, we may apply the techniques of [4] to rewrite these constraints as a differentiable system of nonlinear equations. The key idea is to parameterize the orthogonal matrix of eigenvectors using a *matrix exponential*: as is well known, any orthogonal matrix P with $\det P = 1$ can be represented by[1]

$$P = e^Y = I + Y + \tfrac{1}{2}Y^2 + \cdots,$$

where Y is skew-symmetric, i.e. $Y = -Y^T$. Since eigenvector signs are arbitrary, the assumption that $\det P = 1$ is not a restriction.

Let $\widehat{x}$ be a given point, with the eigenvalues and eigenvectors of $A(\widehat{x})$ given by (1.1)–(1.2). Also, let

$$\widehat{\Lambda}_1 = \mathrm{Diag}(\widehat{\lambda}_1, \ldots, \widehat{\lambda}_t), \quad \widehat{\Lambda}_2 = \mathrm{Diag}(\widehat{\lambda}_{t+1}, \ldots, \widehat{\lambda}_n), \tag{3.7}$$

and let

$$\widehat{Q}_1 = [\widehat{q}_1 \ldots \widehat{q}_t], \quad \widehat{Q}_2 = [\widehat{q}_{t+1} \ldots \widehat{q}_n]. \tag{3.8}$$

Define the twice continuously differentiable $n \times n$ symmetric matrix-valued function

$$\widehat{F}(x, Y, \omega, \Theta) = \begin{bmatrix} \omega I & 0 \\ 0 & \Theta \end{bmatrix} - e^{-Y} \widehat{Q}^T A(x) \widehat{Q} e^Y, \tag{3.9}$$

where $x \in \Re^m$, ω is a real scalar, $\Theta = \mathrm{Diag}(\theta_1, \ldots, \theta_{n-t})$ is a real diagonal matrix of order $n-t$, and Y is a real $n \times n$ skew-symmetric matrix. From

[1] This is easily shown [6] using the spectral decomposition of P, which has eigenvalues of the form ± 1 and $\cos\theta \pm i \sin\theta$, with an even number of -1's.

3 The Matrix Exponential Formulation

Let x^* be a locally unique minimizer of $\phi \equiv \lambda_1$, and let $\lambda_i^* = \lambda_i(x^*)$, $i = 1, \ldots, n$. Suppose that

$$\lambda_1^* = \cdots = \lambda_t^* \ > \ \lambda_{t+1}^* > \cdots > \lambda_n^* \tag{3.1}$$

i.e. the maximum eigenvalue of $A(x^*)$ has multiplicity t, but all other eigenvalues are simple. (The latter assumption usually holds in practice; it could be relaxed, at the cost of more complex notation.) Let

$$\Lambda_1^* = \mathrm{Diag}(\lambda_1^*, \ldots, \lambda_t^*), \quad \Lambda_2^* = \mathrm{Diag}(\lambda_{t+1}^*, \ldots, \lambda_n^*), \tag{3.2}$$

and let $Q^* = [q_1^*, \ldots, q_n^*]$ be a corresponding orthogonal basis of eigenvectors, with

$$Q_1^* = [q_1^* \ldots q_t^*], \quad Q_2^* = [q_{t+1}^* \ldots q_n^*]. \tag{3.3}$$

The matrix Q_2^* is unique, up to the choice of signs for its columns, but the matrix Q_1^* is not, since any particular choice of basis may be rotated by postmultiplying by a $t \times t$ orthogonal matrix.

It was shown in [12] that a necessary condition for x^* to minimize $\phi(x)$ is that there exist a t by t symmetric matrix V^*, with V^* positive semi-definite, such that

$$\mathrm{tr}\ V^* = 1, \quad V^* : \{Q_1^*\}^T [A_x(x^*)\Delta x] Q_1^* = 0, \tag{3.4}$$

for all Δx. In the case $t = 1$, when Q_1^* consists of a single column q_1^*, this reduces to the statement that $\{q_1^*\}^T A_x(x^*)\Delta x] q_1^* = 0$, equivalently $[\phi_x(x^*)\Delta x] = 0$ for all Δx, i.e. the gradient of $\phi(x^*)$ is zero.

We wish to consider the correct local formulation of a Newton-based method so that quadratic convergence to x^* is obtained generically. We assume that the optimal multiplicity t is known. This is not the case in practice, and must be determined during the course of the computation, as explained in [11,12]. If t is set incorrectly, the methods to be described would converge locally to a minimizer of ϕ subject to the wrong multiplicity constraint, which might not be a minimizer of ϕ. This can be avoided, by computing an approximation to V^* and verifying that the necessary conditions for optimality, including the positive semi-definite condition on

and $[A_{xx}\Delta x\Delta x]$ to mean

$$\sum_{k=1}^{m}\sum_{j=1}^{m}\{\Delta x\}_k\{\Delta x\}_j\frac{\partial^2}{\partial x_k\partial x_j}A.$$

We shall reserve square brackets [,] for this purpose, and we shall use parentheses (,) primarily to mean "evaluated at". We shall use braces {, } to indicate expression precedence. For example, the first and second derivatives of $\phi(x)\equiv\lambda_1(x)$ at $x=\widehat{x}$, when $\lambda_1(\widehat{x})$ is simple, given by (1.3)–(1.4), are written in tensor notation as

$$[\phi_x(\widehat{x})\Delta x]=\widehat{q}_1^T[A_x(\widehat{x})\Delta x]\widehat{q}_1$$

and

$$[\phi_{xx}(\widehat{x})\Delta x\Delta x]=\widehat{q}_1^T[A_{xx}\Delta x\Delta x]\widehat{q}_1+2\sum_{s\neq 1}\frac{\{\widehat{q}_1^T[A_x\Delta x]\widehat{q}_s\}^2}{\widehat{\lambda}_1-\widehat{\lambda}_s}.$$

Because the second derivative of a twice continuously differentiable function is symmetric with respect to its two arguments of differentiation, there is no ambiguity in this notation. There should be no confusion between those subscripts indicating differentiation and those indicating components.

We shall use $\|\cdot\|$ to denote the Euclidean vector norm. The expression $A:B$, where A and B are symmetric matrices of the same dimension, means the matrix inner product

$$A:B=\text{tr } AB.$$

The operator "vec" maps the set of symmetric matrices of dimension t into the corresponding vector space $\Re^{t(t+1)/2}$, multiplying the off-diagonal components by the factor $\sqrt{2}$ so that

$$(\text{vec } A)^T(\text{vec } B)=A:B.$$

Consequently

$$\|\text{vec } A\|=\|A\|_F,$$

the Frobenius norm of A.

matrix defined by (1.4). However, it is more often the case that $A(x^*)$ has multiple eigenvalues; this is a consequence of the optimization objective, which in driving all the eigenvalues down as much as possible usually forces the coalescence of some of them. In such a case λ_1 is not generally differentiable at $x = x^*$.

This paper is concerned with the formulation of a Newton-based method to solve optimization problems involving eigenvalues in exactly this case, where multiple eigenvalues occur at the solution. We shall show that the correct problem formulation leads to a method with generic quadratic convergence. This method was first given by [11], inspired in part by [2,4]. Quadratic convergence was demonstrated by numerical examples. The purpose of the present paper is primarily to prove the quadratic convergence property for the method presented in [11], justifying the Hessian matrix formulas given there, which were originally derived only formally and stated without any derivation or proof. The ideas of this paper can be applied to other classes of eigenvalue and singular value optimization problems, e.g. those discussed in [7,12,13,14,17,18], as well as many other references which can be found in these papers. However, we concentrate on the model problem (1.5). For discussion of issues involved in extending these ideas to apply to large-scale problems, see [12].

2 Tensor Notation

We shall have frequent need to refer to the first and second derivatives, with respect to several variables, of matrix-valued functions. Such objects are, respectively, tensors in three and four dimensions, a matrix being a tensor in two dimensions. We shall use subscripts to denote differentiation: thus A_x and A_{xx} refer to the first and second derivatives of the matrix-valued function A, with respect to the variable $x \in \Re^m$. Rather than attempt to describe the elements of a tensor, however, we shall describe its action as a linear operator, the result having the same dimension as the undifferentiated quantity, whether a matrix, a vector, or a scalar. For example, we write $[A_x \Delta x]$ to mean

$$\sum_{k=1}^{m} \{\Delta x\}_k \frac{\partial}{\partial x_k} A$$

The eigenvalues are

$$\lambda_{1,2} = 1 \pm \sqrt{x_1^2 + x_2^2}.$$

Thus λ_1, the largest eigenvalue of $A(x)$, is not generally a smooth function of x; furthermore, it cannot even be written as the maximum of n smooth functions of x, if x has two or more components. Also, the eigenvectors of $A(x)$ cannot generally be written as continuous functions of x; this is a consequence of the fact that eigenvectors corresponding to simple eigenvalues are unique (up to sign and normalization) while those corresponding to multiple eigenvalues are not.

Generally speaking, applications involving eigenvalues of matrices depending on free parameters fall into one of two categories. In the first, it is specified that some or all of the eigenvalues $\lambda_i(x)$ achieve some given values λ_i^*; this is known as an *inverse eigenvalue problem.* If these given values are distinct, the inverse eigenvalue problem may be formulated as a differentiable system of nonlinear equations, and, if the number of free parameters and the number of equations is the same, the application of Newton's method is straightforward, using (1.3). In [4] it was shown how, even in the multiple eigenvalue case, the inverse eigenvalue problem may be formulated as a differentiable system of nonlinear equations, so that Newton-based methods, with generic quadratic convergence, are applicable. This will be explained further below. A key point was to note that the specification of a given eigenvalue with multiplicity t generically imposes $\frac{t(t+1)}{2}$ degrees of restriction on the parameter space, a fact first observed by von Neumann and Wigner in [16].

In the second class of applications, the eigenvalues are not required to have particular values, but rather it is desired to solve some *optimization problem involving the eigenvalues.* A particularly common case is the "min-max" problem

$$\min_{x \in \Re^m} \quad \phi(x) \tag{1.5}$$

where $\phi(x) = \lambda_1(x)$, the largest eigenvalue of $A(x)$. Let x^* be a locally unique minimizer of ϕ. If x^* has the property that the eigenvalue $\lambda_1(x^*)$ is simple, i.e. has multiplicity one, then the function to be minimized, λ_1, is twice continuously differentiable in a neighborhood of x^*, and Newton's method for unconstrained minimization may be applied, using the Hessian

1 Introduction

Let A denote an $n \times n$ real symmetric matrix-valued function depending on a vector of real parameters, $x \in \Re^m$. Assume that A depends smoothly on x, specifically that it is at least twice continuously differentiable, with the second derivative satisfying a Lipschitz condition in x. Denote the eigenvalues of $A(x)$ by

$$\lambda_1(x) \geq \cdots \geq \lambda_n(x).$$

The eigenvalues λ_i are Lipschitz continuous functions of x [8] and, in any region where they are distinct from one another, it is well known that they are (Fréchet) differentiable; in fact, they inherit the C^2 smoothness of the function $A(x)$ [8, p.134]. Let $\widehat{x}$ be given, with

$$A(\widehat{x}) = \widehat{Q}\widehat{\Lambda}\widehat{Q}^T, \quad , \widehat{Q}^T\widehat{Q} = I, \tag{1.1}$$

where

$$\widehat{\Lambda} = \mathrm{Diag}(\widehat{\lambda}_1, \ldots, \widehat{\lambda}_n), \quad \widehat{Q} = [\widehat{q}_1, \ldots, \widehat{q}_n]. \tag{1.2}$$

Thus, $\{\widehat{\lambda}_i\}$ and $\{\widehat{q}_i\}$ are respectively the eigenvalues and an orthonormal set of eigenvectors of $A(\widehat{x})$. Assume that $\widehat{\lambda}_1 \geq \cdots \geq \widehat{\lambda}_n$, so that $\widehat{\lambda}_i = \lambda_i(\widehat{x})$. Then formulas for the first and second partial derivatives of the eigenvalues λ_i at $x = \widehat{x}$, assuming that the $\widehat{\lambda}_i$ are distinct, are

$$\frac{\partial \lambda_i(\widehat{x})}{\partial x_k} = \widehat{q}_i^T \frac{\partial A(\widehat{x})}{\partial x_k} \widehat{q}_i \tag{1.3}$$

and

$$\frac{\partial^2}{\partial x_k \partial x_j} \lambda_i(\widehat{x}) = \widehat{q}_i^T \frac{\partial^2 A(\widehat{x})}{\partial x_k \partial x_j} \widehat{q}_i + 2 \sum_{s \neq i} \frac{\widehat{q}_i^T \frac{\partial A(\widehat{x})}{\partial x_k} \widehat{q}_s \widehat{q}_i^T \frac{\partial A(\widehat{x})}{\partial x_j} \widehat{q}_s}{\widehat{\lambda}_i - \widehat{\lambda}_s}. \tag{1.4}$$

The first of these formulas is well known, and the second may be found in a variety of sources; see [9], [10], as well as (in a somewhat less accessible form) [8, p.95]. Both will follow as special cases of the results given in this paper.

However, if $A(x)$ has multiple eigenvalues at a point $x = \widehat{x}$, its eigenvalues, while still Lipschitz continuous, may not generally be written as differentiable functions of several variables at $x = \widehat{x}$. For example, consider

$$A(x) = \begin{bmatrix} 1 + x_1 & x_2 \\ x_2 & 1 - x_1 \end{bmatrix}.$$

Second Derivatives for Optimizing Eigenvalues of Symmetric Matrices

Michael L. Overton* and Robert S. Womersley†

NYU Computer Science Dept Report 627
March 1993

Abstract

Let A denote an $n \times n$ real symmetric matrix-valued function depending on a vector of real parameters, $x \in \Re^m$. Assume that A is a twice continuously differentiable function of x, with the second derivative satisfying a Lipschitz condition. Consider the following optimization problem: minimize the largest eigenvalue of $A(x)$. Let x^* denote a minimum. Typically, the maximum eigenvalue of $A(x^*)$ is multiple, so the objective function is not differentiable at x^*, and straightforward application of Newton's method is not possible. Nonetheless, the formulation of a Newton-based method with local quadratic convergence is possible. This formulation is derived by parameterizing the eigenvectors using a matrix exponential representation, introducing an appropriate Lagrangian function. Consideration of the Hessian of this Lagrangian function leads to the second derivative matrix used by Newton's method. The derivation of the method and the proof of quadratic convergence take into account the following key fact: the number of variables used in the eigenvector parameterization drops, in the limit, by $t(t-1)/2$, where t is the multiplicity of the maximum eigenvalue of $A(x^*)$. In the special case $t = 1$, the maximum eigenvalue is a smooth function and the method reduces to the standard Newton method. The same ideas are applicable to a wide variety of other eigenvalue and singular value optimization problems.

*Computer Science Department, Courant Institute of Mathematical Sciences, New York University, New York. The work of this author was supported in part by National Science Foundation Grant CCR-9101649. This author would also like to acknowledge the kind hospitality of the Centre for Process Systems Engineering, Imperial College, London, where part of this work was conducted.

†School of Mathematics, University of New South Wales, Australia