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Sensitivity Analysis of the Lanczos Reduction

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For a given real $n \times n$ matrix A and initial vectors v_1 and w_1, we examine the sensitivity of the tridiagonal matrix T and the biorthogonal sets of vectors of the Lanczos reduction to small changes in A, v_1 and w_1. We also consider the sensitivity of the developing Krylov subspaces.

KEY WORDS Lanczos reduction, tridiagonalization, biorthogonalization, Krylov subspace, sensitivity analysis, perturbation analysis, condition

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1. Introduction

Suppose we have been able to tridiagonalize given $A \in \mathcal{R}^{n\times n}$ by a similarity transformation $V^{-1}AV = T$, then with $W \equiv V^{-T}$ for ease of description,

$$AV = VT, \qquad A^T W = WT^T, \qquad W^T V = I, \tag{1.1}$$

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$$W^T A V = T = \begin{pmatrix} \alpha_1 & \gamma_2 & & \\ \beta_2 & \alpha_2 & \cdot & \\ & \cdot & \cdot & \gamma_n \\ & & \beta_n & \alpha_n \end{pmatrix}. \tag{1.2}$$

We will not be concerned so much with how and when such transformations may be obtained, but with how sensitive they are when they exist.

We will examine the sensitivity of V, W and T to small changes in A, $v_1 \equiv Ve_1$ and $w_1 \equiv We_1$, where e_i is the i-th column of the unit matrix I. Sensitivity analyses are of interest in their own right, but there is also a basic numerical motivation for this analysis. For example when A is symmetric we would take $W = V$ orthogonal, corresponding to the symmetric Lanczos tridiagonalization of A with arbitrary unit length v_1 [13], or the direct Givens and Householder tridiagonalizations of A with $v_1 = e_1$, see for example [9, §8.3.1]. Numerically stable implementations of the Givens or Householder reductions lead to computed V_c and T_c such that $(A + \Delta A)\hat{V} = \hat{V}T_c$, $V_c = \hat{V} + \Delta V$, where $\hat{V}$ is orthogonal and $\|\Delta V\|_2 = O(\epsilon)$, $\|\Delta A\|_2/\|A\|_2 = O(\epsilon)$, ϵ being the computer floating point precision, see Wilkinson [18, §§20-28, §§37-45]. Thus a sensitivity analysis would tell us how such ΔA could cause $\hat{V}$, and so V_c, to differ from V, and T_c to differ from T in (1.1).

Because $\kappa_2(V) \equiv \|V\|_2\|V^{-1}\|_2$ can be very large for unsymmetric A, we would normally not want to use (1.1) for such A if a given problem could be solved quickly and accurately some other way. But in some problems we specifically want the T in (1.1). Also if A is large and sparse or structured, whether symmetric or unsymmetric, then the Lanczos algorithm may be a (sometimes the only) feasible approach for finding T, either for itself, or for solving the eigenproblem [13], or for systems of equations [14], see also [10], [16] and [7], or for other practical purposes such as in [8], and for these reasons both the symmetric and unsymmetric Lanczos reductions *are* important.

The sensitivity analysis of (1.1) is also useful in general, in that it not only increases our understanding of what circumstances make the reduction particularly sensitive, and so may help for example in the design and monitoring of algorithms which produce and use the reduction, but it is also an important part of the solution of some problems. The very readable paper [6] by Freund and Feldmann clearly describes the elegant and useful new application of the Lanczos algorithm [8], see also [5], and also shows how the sensitivity of the reduction (1.1) leads to the required sensitivities of the computed results. There it is shown how the sensitivity with respect to some given parameter p can be computed along with the Lanczos vectors in an extended Lanczos algorithm. Here we will treat the more general problem of theoretically describing the overall sensitivity of the factors in (1.1) to any possible small change. From this description condition numbers may also be found.

Work on similar problems was developed by Le and Parlett [15], and by Carpraux, Godunov and Kuznetsov [2]. The relation between this work and those will be discussed in Section 7..

In Section 2. we show why the choice of normalization is important for sensitivity results by discussing some optimality properties of normalizations. In Section 3. we quickly summarize the unsymmetric Lanczos algorithm as background for the sensitivity analysis in Section 4., where the sensitivities of the off-diagonal elements of a matrix Z (which leads to the sensitivities of V and W in (1.1)), diagonal elements of T, and remaining elements of T and Z are developed in separate subsections. The sensitivity results are then summarized in Theorem 4.1. in Section 4.4.. The inverses of two matrices which are critical to the sensitivity are derived in Section 5., and bounds for the general case including Krylov subspaces, and condition numbers for the symmetric case, are derived in Section 6.. The conclusion Section 7. briefly summarizes the work, relates it to similar works, and mentions some of the problems which still need to be treated.

2. Normalization and uniqueness

For any nonsingular diagonal D the forms in (1.1) and (1.2) are preserved when we replace V, W and T by VD, WD^{-1} and $D^{-1}TD$ respectively, so in general we need to specify a normalization to make the reduction unique, and the sensitivity analysis meaningful. But whatever normalization we choose, if $\beta_i\gamma_i \neq 0$, $i = 2, \ldots, k$, but $\beta_{k+1}\gamma_{k+1} = 0$, then the first k columns of V and W, and the leading $k \times k$ block of T will be unique in (1.1) and (1.2) (this can be seen for example from the algorithm (3.7) below), but the rest need not be. This immediately suggests small β_i or γ_i will lead to sensitive reductions, and we will see the analysis supports this later.

To avoid this lack of uniqueness, we will for simplicity assume $\beta_i\gamma_i \neq 0$, $i = 2, \ldots, n$. Since $T - \lambda I$ would then have rank at least $n-1$, this would imply nonderogatory A. However it will be clear from the analysis that when this assumption does not hold, we could analyze the sensitivity of the unique leading parts using the same approach as here.

The normalization will affect the sensitivities, so we discuss the main choices in some detail here. A popular choice, and the one we use here whenever we do specify a normalization, is to take

$$\beta_i = |\gamma_i| > 0, \qquad i = 2, \ldots, n, \tag{2.3}$$

so T becomes what has been called *quasi-symmetric*. This looks like it will minimize some norm of T, which we now show it does. If $D \equiv \mathrm{diag}(\delta_1, \ldots, \delta_n)$ is nonsingular, then transforming T to $D^{-1}TD$ transforms γ_i to $\gamma_i\theta_i$ and β_i to β_i/θ_i where $\theta_i \equiv \delta_i/\delta_{i-1}$, $i = 2, \ldots, n$. The θ_i may be chosen independently, and since $\gamma_i^2\theta_i^2 + \beta_i^2/\theta_i^2$ is minimized when $|\gamma_i\theta_i| = |\beta_i/\theta_i|$, we see the normalization (2.3) *does* minimize $\|T\|_F^2$ (the sum of squares of elements). But we can still have in (1.1) $\|T\|_F = \kappa_2(V)\|A\|_F$, with arbitrarily large $\|T\|_F$ for a given $\|A\|_F$.

This is an unexpected result, so we give an example. Let 2×2 $A_{11} = e_2e_1^T$, and for $0 < \sigma$ define $\Sigma \equiv \mathrm{diag}(1, \sigma)$. With orthogonal Q in the definitions:

$$Q \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \qquad V_{11} \equiv \Sigma Q, \qquad T_{11} \equiv V_{11}^{-1}A_{11}V_{11} = \frac{1}{2\sigma}\begin{pmatrix} -1 & -1 \\ 1 & 1 \end{pmatrix},$$

T_{11} is quasi-symmetric and satisfies $A_{11}V_{11} = V_{11}T_{11}$. If $\sigma \geq 1$ then $1 = \|A_{11}\|_F = \kappa_2(V_{11})\|T_{11}\|_F$, while if $\sigma \leq 1$ then $\|T_{11}\|_F = \sigma^{-1} = \kappa_2(V_{11})\|A_{11}\|_F$, which is arbitrarily large by taking σ arbitrarily small. For $n > 2$ we show how this latter result can be approached arbitrarily closely by extending this example. Let $\sigma < 1$,

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & T_{22} \end{pmatrix}, \quad A_{12} = \begin{pmatrix} \sigma^2 \\ \sigma^3 \end{pmatrix} e_1^T, \quad A_{21} = e_1 \left(\sigma^2 \quad \sigma \right), \quad V = \begin{pmatrix} V_{11} & 0 \\ 0 & I \end{pmatrix},$$

where T_{22} is say σ^2 times a fixed quasi-symmetric tridiagonal matrix, then

$$\begin{aligned} T &\equiv V^{-1}AV = \begin{pmatrix} T_{11} & e_2\sqrt{2}\sigma^2 e_1^T \\ e_1\sqrt{2}\sigma^2 e_2^T & T_{22} \end{pmatrix}, \\ \|T\|_F^2 &= \sigma^{-2} + 4\sigma^4 + \|T_{22}\|_F^2, \quad \kappa_2(V) = \sigma^{-1}, \\ \|A\|_F^2 &= 1 + \sigma^2 + 2\sigma^4 + \sigma^6 + \|T_{22}\|_F^2, \end{aligned}$$

and by decreasing σ we can make $\|T\|_F^2$ arbitrarily large, and $\|T\|_F/[\kappa_2(V)\|A\|_F]$ arbitrarily close to unity.

In our analysis we will consider an instantaneous rate of change $\dot{T}$ of tridiagonal $T(t)$, a differentiable function of scalar t. Since $\dot{T}$ must be tridiagonal, and since $\beta_i(t) = |\gamma_i(t)|$ with the normalization (2.3), we must have $\beta_i^2 = \gamma_i^2$, $2\beta_i\dot{\beta}_i = 2\gamma_i\dot{\gamma}_i$, so multiplying by $\gamma_i/(2\beta_i)$ gives

$$\gamma_i\dot{\beta}_i = \beta_i\dot{\gamma}_i, \tag{2.4}$$

and thus $|\dot{\beta}_i| = |\dot{\gamma}_i|$, meaning $\dot{T}$ is also quasi-symmetric, and so also has minimum F-norm over all nonsingular diagonal D. Thus (2.3) is an attractive normalization to take when examining the sensitivity of T alone, as it introduces no spurious sensitivity. More arbitrary normalizations such as $\beta_i = 1$ are clearly much less appealing for this analysis.

Other normalizations concentrate on the sizes of the columns v_i and w_i of V and W in (1.1), while ensuring $w_i^T v_i = 1$. For fixed $\hat{V}$ and $\hat{W}$ consider $V = \hat{V}D$ and $W = \hat{W}D^{-1}$ in $\kappa(V) = \|V\|.\|W^T\|$. Differentiating $\kappa_F^2(V)$ with respect to the elements of D shows its minimum occurs when

$$\|w_i\|_2 = \|v_i\|_2, \qquad i = 1, \ldots, n, \tag{2.5}$$

so this normalization could be used when the F-norm condition of V is the major concern. Finally if D_2 equilibrates the columns of $V = \hat{V}D_2$ in the sense that for every column $\|v_i\|_2 = 1$, and if $D = D_{min}$ minimizes $\kappa_2(\hat{V}D)$, then van der Sluis [17, Thm. 3.5] showed

$$\kappa_2(\hat{V}D_{min}) \le \kappa_2(\hat{V}D_2) \le \sqrt{n}\kappa_2(\hat{V}D_{min}),$$

and so either the normalization $\|v_i\|_2 = 1$, $i = 1, \ldots, n$, or the equivalent normalization for W, will give a good approximation to minimizing $\kappa_2(V)$.

If we used (2.3), we could later compute $D_F = \mathrm{diag}(\sqrt{\|w_i\|_2/\|v_i\|_2})$ so $\kappa_F(VD_F)$ is the minimum of $\kappa_F(VD)$, and then we would know

$$\kappa_F(V) \ge \kappa_F(VD_F) \ge \kappa_F(V)/\kappa_2(D_F),$$

so $\kappa_2(D_F)$ would indicate how far $\kappa_F(V)$ could be from the minimum with respect to diagonal D of $\kappa_F(VD)$.

For symmetric A, the normalizations (2.3), (2.5), $\|v_i\|_2 = 1$, and $\|w_i\|_2 = 1$, (each with $W^TV = I$) all give symmetric T and orthogonal $W = V$.

3. The unsymmetric Lanczos algorithm

The unsymmetric Lanczos algorithm (in theory) develops the reduction (1.1) as follows. Here we use the normalization in (2.3). Assume we are given

$$A, \quad v_1 \text{ and } w_1 \text{ such that } w_1^T v_1 = 1. \tag{3.6}$$

Set $\alpha_1 = w_1^T A v_1$, $\bar{v}_2 = Av_1 - \alpha_1 v_1$, $\bar{w}_2 = A^T w_1 - \alpha_1 w_1$. For $i = 2, 3, \ldots, n$ the general step is then:

If $\bar{v}_i = 0$ or $\bar{w}_i = 0$ or $\bar{w}_i^T \bar{v}_i = 0$ STOP.

Otherwise choose $\beta_i = |\gamma_i|$ such that $\beta_i v_i = \bar{v}_i$, $\gamma_i w_i = \bar{w}_i$, $w_i^T v_i = 1$,

$$\begin{aligned} \alpha_i &= w_i^T A v_i, \\ \bar{v}_{i+1} &= Av_i - \alpha_i v_i - \gamma_i v_{i-1}, \\ \bar{w}_{i+1} &= A^T w_i - \alpha_i w_i - \beta_i w_{i-1}. \end{aligned} \tag{3.7}$$

Biorthogonality of the w_i and v_i can easily be proven recursively. If the algorithm does not stop prematurely, so that it ceases only after step $i = n$, then (2.3) holds, $W^TV = I$, and we must have here $\bar{v}_{n+1} = 0$ and $\bar{w}_{n+1} = 0$, and (1.1) follows. Of course (3.7) also follows simply from observing the columns of (1.1) and the diagonal elements of (1.2).

4. Sensitivity analysis

Suppose the Lanczos algorithm (3.7) applied to A with starting vectors v_1 and w_1 does not stop prematurely, and gives (1.1) and (1.2) with (2.3). Let $A(t) \in \mathcal{R}^{n \times n}$ and $v_1(t), w_1(t) \in \mathcal{R}^n$ be differentiable functions of scalar t with

$$A(0) = A, \quad v_1(0) = v_1, \quad w_1(0) = w_1, \quad v_1(t)^T w_1(t) = 1. \tag{4.8}$$

Here we could define $A(t) \equiv A + t\Delta A$ for arbitrary but small ΔA, which suggests we can also handle structured perturbations, perhaps considering changes in only a few elements of A. Since $v_1(t)^T w_1(t) = 1$, similar linear functions could be too restrictive for $v_1(t)$ and $w_1(t)$. Often we will just be interested in the sensitivity with respect to changes in A, and then we will take $\dot{v}_1 = \dot{w}_1 = 0$, but the basic analysis is no more difficult with them nonzero. If we carry out the Lanczos algorithm (3.6) and (3.7) with these functions, an examination of the algorithm shows each function is differentiable while the $\beta_i(t)\gamma_i(t) \neq 0$, so since (2.3) holds, for small enough t the algorithm will not stop prematurely, and the resulting functions will satisfy the equivalents of (1.1) and (1.2)

$$\begin{aligned} A(t)V(t) &= V(t)T(t), \qquad & A(t)^T W(t) &= W(t)T^T(t), \\ W(t)^T V(t) &= I, \qquad & W(t)^T A(t) V(t) &= T(t). \end{aligned} \tag{4.9}$$

The same can be shown for any other unique choice of normalization. We will derive expressions for the derivatives at $t = 0$, and write $\dot{A} \equiv \dot{A}(0)$, $\dot{V} \equiv \dot{V}(0)$ *etc.* for simplicity.

Differentiating these last two equations at $t = 0$ gives

$$W^T\dot{V} + \dot{W}^T V = 0, \qquad W^T A\dot{V} + \dot{W}^T AV + W^T\dot{A}V = \dot{T}.$$

But $W^TA = TW^T$, $AV = VT$, and writing

$$Z_0 \equiv -W^T\dot{V} = \dot{W}^T V, \qquad M_A \equiv W^T\dot{A}V, \tag{4.10}$$

gives the crucial relationship

$$\dot{T} + TZ_0 - Z_0T = M_A. \tag{4.11}$$

We will see both $\dot{T}$ and $Z_0 = -W^T\dot{V} = \dot{W}^T V$ can be developed from this one matrix equation, and then

$$\begin{aligned} \dot{V} &= -W^{-T}Z_0 = -VZ_0, \\ \dot{W} &= V^{-T}Z_0^T = WZ_0^T. \end{aligned} \tag{4.12}$$

The key is to remember that like T, $\dot{T}$ must be tridiagonal, and since $\dot{v}_1$ and $\dot{w}_1$ are known, Z_0 has known first column $-W^T\dot{v}_1$ and row $\dot{w}_1^T V$. Write $Z_0 = Z_1 + Z$ where Z_1 is the known, and Z the unknown part of Z_0, Z having zero first row and column. This gives for (4.11)

$$\dot{T} + TZ - ZT = M_A - TZ_1 + Z_1T \equiv M, \quad \text{say, with structure:} \tag{4.13}$$

$$\begin{aligned} &\begin{pmatrix} \dot\alpha_1 & \dot\gamma_2 & & \\ \dot\beta_2 & \dot\alpha_2 & \cdot & \\ & \cdot & \cdot & \dot\gamma_n \\ & & \dot\beta_n & \dot\alpha_n \end{pmatrix} + \begin{pmatrix} \alpha_1 & \gamma_2 & & \\ \beta_2 & \alpha_2 & \cdot & \\ & \cdot & \cdot & \gamma_n \\ & & \beta_n & \alpha_n \end{pmatrix} \begin{pmatrix} 0 & & & \\ & z_{22} & \cdot & z_{2n} \\ & \cdot & \cdot & \cdot \\ & z_{n2} & \cdot & z_{nn} \end{pmatrix} \\ &\qquad - \begin{pmatrix} 0 & & & \\ & z_{22} & \cdot & z_{2n} \\ & \cdot & \cdot & \cdot \\ & z_{n2} & \cdot & z_{nn} \end{pmatrix} \begin{pmatrix} \alpha_1 & \gamma_2 & & \\ \beta_2 & \alpha_2 & \cdot & \\ & \cdot & \cdot & \gamma_n \\ & & \beta_n & \alpha_n \end{pmatrix} \\ &\qquad = M. \end{aligned} \tag{4.14}$$

This structure allows us to split the sensitivity problem into manageable subproblems. First we will show how to obtain one nonsingular triangular linear system whose solution contains all the subdiagonal elements of Z, and an independent one giving the above-diagonal elements. Next we will see there is a simple expression for each diagonal element of $\dot{T}$. The diagonal elements of Z are zero in the case of symmetric A and $\dot{A}$, but the unsymmetric case is more challenging: note (4.14) is n^2 linear equations in the $(n-1)^2 + 3n - 2$ unknown elements of Z and $\dot{T}$, so we need $n-1$ more equations. Specifying the particular normalization used gives the required number, and we will use (2.3) in the form of (2.4).

4.1. Off-diagonal elements of Z

The off-diagonal elements of Z can be found independently of the other elements of Z or of $\dot{T}$. We show how to find the strictly lower triangle of Z. Elements 3 to n of the 1st column of (4.14) give

$$-\beta_2 I \begin{pmatrix} z_{32} \\ \cdot \\ z_{n2} \end{pmatrix} = \begin{pmatrix} m_{31} \\ \cdot \\ m_{n1} \end{pmatrix},$$

then elements 4 to n of the 2nd column give

$$-\alpha_2 I \begin{pmatrix} z_{42} \\ \cdot \\ z_{n2} \end{pmatrix} - \beta_3 I \begin{pmatrix} z_{43} \\ \cdot \\ z_{n3} \end{pmatrix} + \begin{pmatrix} \beta_4 & \alpha_4 & \gamma_5 & \\ & \cdot & \cdot & \cdot \\ & & \beta_n & \alpha_n \end{pmatrix} \begin{pmatrix} z_{32} \\ \cdot \\ z_{n2} \end{pmatrix} = \begin{pmatrix} m_{42} \\ \cdot \\ m_{n2} \end{pmatrix},$$

while for $i = 3, 4, \ldots, n-2$, elements $i+2$ to n of the ith column give

$$\begin{aligned} - \quad & \gamma_i I \begin{pmatrix} z_{i+2,i-1} \\ \cdot \\ z_{n,i-1} \end{pmatrix} - \alpha_i I \begin{pmatrix} z_{i+2,i} \\ \cdot \\ z_{n,i} \end{pmatrix} - \beta_{i+1} I \begin{pmatrix} z_{i+2,i+1} \\ \cdot \\ z_{n,i+1} \end{pmatrix} \\ + \quad & \begin{pmatrix} \beta_{i+2} & \alpha_{i+2} & \gamma_{i+3} & \\ & \cdot & \cdot & \cdot \\ & & \beta_n & \alpha_n \end{pmatrix} \begin{pmatrix} z_{i+1,i} \\ \cdot \\ z_{n,i} \end{pmatrix} = \begin{pmatrix} m_{i+2,i} \\ \cdot \\ m_{n,i} \end{pmatrix}. \end{aligned}$$

By using standard MATLAB notation for subscripts, so that for example $m_{i:j,k}$ represents the column vector of elements i to j in column k of M, we may write the above in block form as

$$L \begin{pmatrix} z_{3:n,2} \\ z_{4:n,3} \\ z_{5:n,4} \\ \cdot \\ z_{i+2:n,i+1} \\ \cdot \\ z_{n,n-1} \end{pmatrix} = \begin{pmatrix} m_{3:n,1} \\ m_{4:n,2} \\ m_{5:n,3} \\ \cdot \\ m_{i+2:n,i} \\ \cdot \\ m_{n,n-2} \end{pmatrix}, \tag{4.15}$$

where $L = L(T)$ is the $n-2$ block by $n-2$ block lower triangular matrix

$$-\begin{pmatrix} \beta_2 I_{n-2} & & & & & \\ B_2 & \beta_3 I_{n-3} & & & & \\ [0,0,\gamma_3 I_{n-4}] & B_3 & \beta_4 I_{n-4} & & & \\ & \cdot & \cdot & \cdot & & \\ & & [0,0,\gamma_i I_{n-i-1}] & B_i & \beta_{i+1} I_{n-i-1} & \\ & & & \cdot & \cdot & \cdot \\ & & & [0,0,\gamma_{n-2}] & B_{n-2} & \beta_{n-1} \end{pmatrix}, \tag{4.16}$$

with $B_i \equiv [\alpha_i I - T]_{i+2:n,i+1:n}$, $i = 2, 3, \ldots, n-2$.

By analogy, transposing (4.13) to give $\dot{T}^T - T^T Z^T + Z^T T^T = M^T$ gives for the strictly upper triangle of Z (using $m_{k,i:j}$ to represent the row vector of elements i

to j in row k of M, and $m^T_{k,i:j}$ its transpose, and noting $[Z^T]_{i:j,k} = z^T_{k,i:j}$)

$$U^T \begin{pmatrix} z^T_{2,3:n} \\ z^T_{3,4:n} \\ z^T_{4,5:n} \\ \cdot \\ z^T_{i+1,i+2:n} \\ \cdot \\ z_{n-1,n} \end{pmatrix} = \begin{pmatrix} m^T_{1,3:n} \\ m^T_{2,4:n} \\ m^T_{3,5:n} \\ \cdot \\ m^T_{i,i+2:n} \\ \cdot \\ m_{n-2,n} \end{pmatrix}, \tag{4.17}$$

where $U^T = U(T)^T$ is the $n-2$ block by $n-2$ block nonsingular lower triangular matrix

$$\begin{pmatrix} \gamma_2 I_{n-2} & & & & & & \\ G_2 & \gamma_3 I_{n-3} & & & & & \\ [0,0,\beta_3 I_{n-4}] & G_3 & \gamma_4 I_{n-4} & & & & \\ & \cdot & \cdot & \cdot & & & \\ & & [0,0,\beta_i I_{n-i-1}] & G_i & \gamma_{i+1} I_{n-i-1} & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & [0,0,\beta_{n-2}] & G_{n-2} & \gamma_{n-1} \end{pmatrix}, \tag{4.18}$$

with $G_i \equiv [\alpha_i I - T^T]_{i+2:n,i+1:n}$, $i = 2, 3, \ldots, n-2$. Note with the normalization (2.3) we have quasi-symmetric T, and so

$$|U^T| = |L|. \tag{4.19}$$

4.2. *Diagonal elements of $\dot{T}$*

It is pleasing that the problem splits into finding the elements in the strictly lower and upper triangular parts of Z sequentially, with the lower independent of the upper and of the other unknowns. This easy development continues, for we may now find the $\dot{\alpha}_i$ in terms of the next to (or second) diagonal elements of Z and the diagonal elements of M alone. From the diagonal elements of (4.14)

$$\begin{aligned} \dot{\alpha}_1 &= m_{11}, \\ \dot{\alpha}_2 &= m_{22} + \beta_3 z_{23} - \gamma_3 z_{32}, \\ \dot{\alpha}_i &= m_{ii} + \gamma_i z_{i,i-1} - \beta_i z_{i-1,i} + \beta_{i+1} z_{i,i+1} - \gamma_{i+1} z_{i+1,i}, \\ & \qquad i = 3, 4, \ldots, n-1, \\ \dot{\alpha}_n &= m_{nn} + \gamma_n z_{n,n-1} - \beta_n z_{n-1,n}. \end{aligned} \tag{4.20}$$

4.3. *The remaining elements of $\dot{T}$ and Z*

The *analysis* so far has been independent of the normalization chosen, though the actual *values* will still depend on the normalization used. But now we need to specify the normalization in order to obtain separate expressions for the off-diagonal elements of $\dot{T}$, and for the diagonal elements of Z. For the reasons stated in Section 2. we assume (2.3), giving (2.4).

Since $\beta_i = \pm\gamma_i$, we can take $D \equiv \mathrm{diag}(1, \delta_2, \ldots, \delta_n)$ with $\delta_i = \delta_{i-1}\beta_i/\gamma_i$, $i =$

$2,\ldots,n$, so TD and $\dot{T}D$ are symmetric. Let $Z_D \equiv \mathrm{diag}(z_{11},\ldots,z_{nn})$, $z_{11}=0$, $\bar{Z} \equiv Z - Z_D$, then from (4.13)

$$\begin{aligned} \dot{T} &= M + ZT - TZ = N + S, \\ N &\equiv M + \bar{Z}T - T\bar{Z}, \qquad S \equiv Z_D T - T Z_D, \end{aligned} \tag{4.21}$$

where N can be computed at this stage. Note $SD = Z_D TD - TZ_D D = Z_D TD - TDZ_D$, and SD is skew symmetric since $(SD)^T = TDZ_D - Z_D TD = -SD$.

Since $\dot{T}D = ND + SD$ is symmetric with SD skew symmetric, taking the transpose of each side of the former and adding gives

$$\dot{T} = \tfrac{1}{2}(DN^T D^{-1} + N), \qquad N \equiv M + \bar{Z}T - T\bar{Z}, \qquad |D| = I, \tag{4.22}$$

which does not depend on Z_D. If instead of adding we subtract, we get

$$S = \tfrac{1}{2}(DN^T D^{-1} - N). \tag{4.23}$$

We will use these matrix expressions in Section 6..

We now define ζ_i and η_i so that the following two equations easily fit in with (4.16) and (4.18). This simplifies the presentation of Theorem 1 in the next section. From (4.21)

$$-\beta_i\zeta_i \equiv n_{i,i-1} = m_{i,i-1} + \gamma_{i-1}z_{i,i-2} + (\alpha_{i-1}-\alpha_i)z_{i,i-1} - \gamma_{i+1}z_{i+1,i-1}, \tag{4.24}$$

$$\gamma_i\eta_i \equiv n_{i-1,i} = m_{i-1,i} - \beta_{i-1}z_{i-2,i} - (\alpha_{i-1}-\alpha_i)z_{i-1,i} + \beta_{i+1}z_{i-1,i+1}, \tag{4.25}$$

where we use $z_{1j} = z_{j1} = 0$ for $j = 1,\ldots,n$ and define $\beta_1 = \gamma_1 = \beta_{n+1} = \gamma_{n+1} = 0$ so these definitions hold for $i = 2,\ldots,n$. With these, and remembering $\delta_i = \delta_{i-1}\beta_i/\gamma_i$, the $(i,i-1)$ and $(i-1,i)$ elements of (4.22) give for $i = 2,\ldots,n$

$$\dot{\beta}_i = (\delta_i\delta_{i-1}^{-1}n_{i-1,i} + n_{i,i-1})/2 = \beta_i(\eta_i - \zeta_i)/2, \tag{4.26}$$

$$\dot{\gamma}_i = (\delta_{i-1}\delta_i^{-1}n_{i,i-1} + n_{i-1,i})/2 = \gamma_i(\eta_i - \zeta_i)/2, \tag{4.27}$$

while the $(i,i-1)$ element of (4.23), with (4.21), gives

$$\beta_i(z_{ii} - z_{i-1,i-1}) = (\delta_i\delta_{i-1}^{-1}n_{i-1,i} - n_{i,i-1})/2 = \beta_i(\eta_i + \zeta_i)/2,$$

so for $i = 2,\ldots,n$ with $z_{11} = 0$

$$z_{ii} = z_{i-1,i-1} + (\eta_i + \zeta_i)/2, \tag{4.28}$$

which completes the expressions for the sensitivities.

4.4. Summary of the sensitivity expressions

The sensitivity results we have so far derived can be summarized as follows.

Theorem 4.1. *Let $A(t) \in \mathcal{R}^{n\times n}$ and $v_1(t), w_1(t) \in \mathcal{R}^n$ be (known) differentiable functions of scalar t with*

$$A(0) = A, \quad v_1(0) = v_1, \quad w_1(0) = w_1, \quad v_1(t)^T w_1(t) = 1,$$

such that the Lanczos algorithm (3.6)–(3.7) applied to A *with starting vectors* v_1 *and* w_1 *leads to tridiagonal* T *where*

$$AV = VT, \qquad W^T V = I, \qquad T = \begin{pmatrix} \alpha_1 & \gamma_2 & & \\ \beta_2 & \alpha_2 & \cdot & \\ & \cdot & \cdot & \gamma_n \\ & & \beta_n & \alpha_n \end{pmatrix},$$

$$V = [v_1, \ldots, v_n], \quad W = [w_1, \ldots, w_n], \quad \beta_i = |\gamma_i| > 0, \quad i = 2, \ldots, n. \tag{4.29}$$

Then for t *close enough to zero the Lanczos algorithm (3.6)–(3.7) applied to* $A(t)$ *with starting vectors* $v_1(t)$ *and* $w_1(t)$ *leads to*

$$A(t)V(t) = V(t)T(t), \qquad W(t)^T V(t) = I, \tag{4.30}$$

$$T(t) = \begin{pmatrix} \alpha_1(t) & \gamma_2(t) & & \\ \beta_2(t) & \alpha_2(t) & \cdot & \\ & \cdot & \cdot & \gamma_n(t) \\ & & \beta_n(t) & \alpha_n(t) \end{pmatrix},$$

$$\beta_i(t) = |\gamma_i(t)| > 0, \qquad i = 2, \ldots, n, \tag{4.31}$$

with each function differentiable and $T(0) = T$, $V(0) = V$, $W(0) = W$. *If we write* $\dot{A} \equiv \dot{A}(0)$ etc., *and define (known)* Z_1 *such that*

$$[Z_1]_{2:n,2:n} = 0, \qquad Z_1 e_1 = -W^T \dot{v}_1, \qquad e_1^T Z_1 = \dot{w}_1^T V, \tag{4.32}$$

then the instantaneous rates of change $\dot{V}$ *and* $\dot{W}$ *satisfy*

$$\dot{V} = -V(Z_1 + Z), \qquad \dot{W} = W(Z_1 + Z)^T, \tag{4.33}$$

where $Ze_1 = 0$, $e_1^T Z = 0$, *and* $\dot{T}$, Z *are otherwise uniquely determined by*

$$\dot{T} + TZ - ZT = M \equiv W^T \dot{A} V - TZ_1 + Z_1 T. \tag{4.34}$$

Part of (4.34) can be written as a matrix-vector equation for the scalars ζ_j *and the strictly lower triangular elements* $z_{j+1:n,j}$, $j = 2, \ldots, n-1$, *of* Z:

$$\tilde{L} \begin{pmatrix} \tilde{z}_2 \\ \cdot \\ \tilde{z}_{n-1} \\ \zeta_n \end{pmatrix} = \begin{pmatrix} m_{2:n,1} \\ \cdot \\ m_{n-1:n,n-2} \\ m_{n,n-1} \end{pmatrix}; \qquad \tilde{z}_j \equiv \begin{pmatrix} \zeta_j \\ z_{j+1:n,j} \end{pmatrix}, \quad j = 2, \ldots, n-1, \tag{4.35}$$

where $\tilde{L} = \tilde{L}(T)$ *is the* $n-1$ *block by* $n-1$ *block lower triangular matrix*

$$-\begin{pmatrix} \beta_2 I_{n-1} & & & & & \\ [0, \tilde{B}_2] & \beta_3 I_{n-2} & & & & \\ [0,0,\gamma_3 I_{n-3}] & [0, \tilde{B}_3] & \beta_4 I_{n-3} & & & \\ \cdot & \cdot & \cdot & & & \\ & & [0,0,\gamma_i I_{n-i}] & [0, \tilde{B}_i] & \beta_{i+1} I_{n-i} & \\ & & \cdot & \cdot & \cdot & \\ & & & [0,0,\gamma_{n-1}] & [0, \tilde{B}_{n-1}] & \beta_n \end{pmatrix}, \tag{4.36}$$

where the (i,j)-block is $n-i \times n-j$, and for $i = 2,3,\ldots,n-1$

$$\tilde{B}_i \equiv [\alpha_i I - T]_{i+1:n,i+1:n} = \begin{pmatrix} \alpha_i - \alpha_{i+1} & -\gamma_{i+2} & & \\ -\beta_{i+2} & \alpha_i - \alpha_{i+2} & \cdot & \\ & \cdot & \cdot & -\gamma_n \\ & & -\beta_n & \alpha_i - \alpha_n \end{pmatrix}. \tag{4.37}$$

Another part of (4.34) supplies an equation for the scalars η_j and the strictly upper part $z_{j,j+1:n}$, $j = 2,\ldots,n-1$, of Z:

$$\tilde{U}^T \begin{pmatrix} \tilde{y}_2 \\ \cdot \\ \tilde{y}_{n-1} \\ \eta_n \end{pmatrix} = \begin{pmatrix} m^T_{1,2:n} \\ \cdot \\ m^T_{n-2,n-1:n} \\ m_{n-1,n} \end{pmatrix}; \qquad \tilde{y}_j \equiv \begin{pmatrix} \eta_j \\ z^T_{j,j+1:n} \end{pmatrix}, \ j = 2,\ldots,n-1, \tag{4.38}$$

where $\tilde{U}^T = \tilde{U}(T)^T$ is the $n-1$ block by $n-1$ block lower triangular matrix

$$\begin{pmatrix} \gamma_2 I_{n-1} & & & & & \\ [0,\tilde{B}_2^T] & \gamma_3 I_{n-2} & & & & \\ [0,0,\beta_3 I_{n-3}] & [0,\tilde{B}_3^T] & \gamma_4 I_{n-3} & & & \\ \cdot & \cdot & \cdot & & & \\ & [0,0,\beta_i I_{n-i}] & [0,\tilde{B}_i^T] & \gamma_{i+1} I_{n-i} & & \\ & & \cdot & \cdot & \cdot & \\ & & & [0,0,\beta_{n-1}] & [0,\tilde{B}_{n-1}^T] & \gamma_n \end{pmatrix}. \tag{4.39}$$

The additional elements ζ_j and η_j in (4.35) and (4.38) give the diagonal elements of Z:

$$z_{jj} = \frac{1}{2}\sum_{i=2}^{j}(\zeta_i + \eta_i), \qquad j = 2,3,\ldots,n, \tag{4.40}$$

and the next to diagonal elements of $\dot{T}$:

$$\dot{\beta}_j/\beta_j = \dot{\gamma}_j/\gamma_j = \tfrac{1}{2}(\eta_j - \zeta_j), \qquad j = 2,3,\ldots,n. \tag{4.41}$$

The diagonal elements of $\dot{T}$ can be found from the diagonal elements of M and the next to diagonal elements of Z, where if we use $z_{1i} = z_{i1} = 0$ for $i = 1,\ldots,n$, and define $\beta_1 = \gamma_1 = \beta_{n+1} = \gamma_{n+1} = 0$,

$$\dot{\alpha}_i = m_{ii} + \gamma_i z_{i,i-1} - \beta_i z_{i-1,i} + \beta_{i+1} z_{i,i+1} - \gamma_{i+1} z_{i+1,i}, \quad i = 1,\ldots,n. \tag{4.42}$$

These two expressions for the elements of $\dot{T}$ can be summarized as

$$\dot{T} = \tfrac{1}{2}(DN^TD^{-1} + N), \qquad N \equiv M + \bar{Z}T - T\bar{Z}, \qquad |D| = I, \tag{4.43}$$

where $\bar{Z}$ is Z with its diagonal made zero.

Proof The existence of the unique reduction (4.30) with (4.31) follows from the discussion at the start of Section 4., while (4.32) to (4.34) follow from (4.10) to (4.13). The linear system (4.35) to (4.37) is just (4.15) and (4.16) with the addition of equations (4.24) (with its equivalents for $i = 2,3,n$) and unknowns $\zeta_2,\ldots,\zeta_n$.

The linear system (4.38) with (4.39) is the equivalent of (4.35) to (4.37), but now for the strictly upper triangle of Z and $\eta_2, \ldots, \eta_n$. It can be found by applying those ideas to $\dot{T}^T - T^T Z^T + Z^T T^T = M^T$. Next (4.40) follows from (4.28) and $z_{11} = 0$, (4.41) follows from (4.26) and (4.27), and (4.42) follows from (4.20). The matrix version (4.43) is just (4.22). ∎

Corollary 1 *If any other normalization than that in (4.29) is used, all the results of the theorem hold except (4.31), (4.40), (4.41) and (4.43). These would have to be altered to suit the particular normalization, see Section 2..* ∎

Corollary 2 *In (4.36) the column below the leading element of each diagonal block* $(\beta_i I_{n-i+1})$ *is zero, with a similar observation for (4.39). Thus the off-diagonal elements of* Z *can be computed without computing the* ζ_i *and* η_i*, see (4.35) and (4.38).* ∎

5. Expressions for the inverses

To bound the elements of Z in (4.35) and (4.38) it will help to know the inverse of L, the submatrix obtained by dropping the first row and column of each diagonal block of $\tilde{L}$, see (4.16), and U^T, the equivalent submatrix of $\tilde{U}^T$. These inverses can be expressed in terms of polynomials in T and T^T. We have from (1.2)

$$T_{j+1:i,j+1:i} = \begin{pmatrix} \alpha_{j+1} & \gamma_{j+2} & & \\ \beta_{j+2} & \alpha_{j+2} & \cdot & \\ & \cdot & \cdot & \gamma_i \\ & & \beta_i & \alpha_i \end{pmatrix}.$$

For $j = 0, \ldots, n-1$ define the polynomials in λ

$$\varphi_j^{(j)}(\lambda) \equiv 1, \tag{5.44}$$

$$\varphi_i^{(j)}(\lambda) \equiv \det([\lambda I - T]_{j+1:i,j+1:i}), \quad i = j+1, \ldots, n, \tag{5.45}$$

so $\varphi_i^{(j)}(\lambda)$ is monic and has degree $i - j$ in λ, and its zeros are the eigenvalues of $T_{j+1:i,j+1:i}$. We see

$$\varphi_{j+1}^{(j)}(\lambda) = \lambda - \alpha_{j+1}, \tag{5.46}$$

$$\varphi_i^{(j)}(\lambda) = (\lambda - \alpha_i)\varphi_{i-1}^{(j)}(\lambda) - \beta_i \gamma_i \varphi_{i-2}^{(j)}(\lambda), \quad i = j+2, \ldots, n. \tag{5.47}$$

The inverse of L can be expressed in terms of the $\varphi_i^{(j)}(T)$, and that of U^T in terms of the $\varphi_i^{(j)}(T^T)$. Note from (5.44) $\varphi_j^{(j)}(T) = \varphi_j^{(j)}(T^T) = I$, while for $i > j$, $\varphi_i^{(j)}(T)$ and $\varphi_i^{(j)}(T^T)$ can be found from (5.46) and (5.47).

Theorem 5.1. *Let T be as in (1.2), and $\varphi_i^{(j)}(\lambda)$ as in (5.44)–(5.45). Let $X \equiv L^{-1}$ be partitioned identically as L in (4.16), with $n-i-1$ by $n-j-1$ X_{ij} its (i,j) block. Then for $j = 1, 2, \ldots, n-2$ and $i = j, \ldots, n-2$*

$$X_{ij} = -(\beta_{j+1}\beta_{j+2} \cdots \beta_{i+1})^{-1} \varphi_i^{(j)}(T)_{i+2:n,j+2:n}. \tag{5.48}$$

Proof Since the j-th block-column of $LX = I$ is

$$L[0,\ldots,0,X_{jj}^T,X_{j+1,j}^T,\ldots,X_{n-2,j}^T]^T = [0,\ldots,0,I_{n-j-1},0,\ldots,0]^T,$$

the form of L in (4.16), with (5.44), shows (5.48) holds with $i=j$. Also

$$X_{j+1,j} = -\beta_{j+2}^{-1}B_{j+1}X_{jj} = -(\beta_{j+1}\beta_{j+2})^{-1}(T-\alpha_{j+1}I)_{j+3:n,j+2:n},$$

which with (5.46) satisfies (5.48). If (5.48) is true for $i=j,\ldots,k-1$, then

$$\begin{aligned} X_{kj} &= -\beta_{k+1}^{-1}\{B_kX_{k-1,j} + [0,0,\gamma_kI_{n-k-1}]X_{k-2,j}\} \\ &= -\beta_{k+1}^{-1}\{-(\beta_{j+1}\cdots\beta_k)^{-1}(\alpha_kI-T)_{k+2:n,k+1:n}\varphi_{k-1}^{(j)}(T)_{k+1:n,j+2:n} \\ &\qquad -(\beta_{j+1}\cdots\beta_{k-1})^{-1}[0,0,\gamma_kI_{n-k-1}]\varphi_{k-2}^{(j)}(T)_{k:n,j+2:n}\} \\ &= -(\beta_{j+1}\cdots\beta_{k+1})^{-1}\{(T-\alpha_kI)_{k+2:n,k+1:n}\varphi_{k-1}^{(j)}(T)_{k+1:n,j+2:n} \\ &\qquad\qquad -\beta_k\gamma_k\varphi_{k-2}^{(j)}(T)_{k+2:n,j+2:n}\}. \end{aligned}$$

But $(T-\alpha_kI)_{k+2:n,k+1:n}\varphi_{k-1}^{(j)}(T)_{k+1:n,j+2:n} = [T-(\alpha_kI)\varphi_{k-1}^{(j)}(T)]_{k+2:n,j+2:n}$ since each row of $(T-\alpha_kI)_{k+2:n,k+1:n}$ has the same *nonzeros* as each corresponding row of α_kI-T. Using (5.47) we see (5.48) then holds for $i=k$, and by induction for $i=j,\ldots,n-2$. ■

Corollary 3 *Let U^T be the matrix obtained by dropping the first row and column of each diagonal block of $\tilde{U}^T$ in (4.39), see (4.18). If $Y\equiv U^{-T}$ is partitioned identically to U^T, with $n-i-1$ by $n-j-1$ Y_{ij} its (i,j) block, then for $j=1,2,\ldots,n-2$ and $i=j,\ldots,n-2$*

$$Y_{ij} = (\gamma_{j+1}\gamma_{j+2}\cdots\gamma_{i+1})^{-1}\varphi_i^{(j)}(T^T)_{i+2:n,j+2:n}. \tag{5.49}$$

Proof The proof is analogous to that for L^{-1}. ■

Note with (2.3) $|(\gamma_{j+1}\cdots\gamma_{i+1})^{-1}| = (\beta_{j+1}\cdots\beta_{i+1})^{-1}$, also $\varphi_i^{(j)}(T^T) = \varphi_i^{(j)}(T)^T$, but in general $Y_{ij} \neq \pm X_{ij}$.

6. Condition numbers and bounds

Theorem 4.1. gives all the basics needed to understand the sensitivity of the reduction. From this we can produce various element and norm bounds and condition numbers. Here we will illustrate this by giving some basic norm bounds and condition numbers. Because of lack of time to develop them carefully, the bounds in the unsymmetric case are probably unnecessarily weak. We will not do the analysis for W, since from (1.1), the parallel with that for V is obvious.

First we indicate how this work is related to perturbation bounds. Suppose we have some differentiable factor $N(t)$ of $A(t)$ and are able to prove

$$\frac{\|\dot{N}(0)\|_\alpha}{\|N\|_\beta} \le \kappa\frac{\|\dot{A}(0)\|_\gamma}{\|A\|_\delta},$$

where κ is a function of A, the reduction, and the norms chosen (denoted by $\alpha, \beta, \gamma, \delta$ here), and suppose for any $A = A(0)$ having a unique reduction that equality may be obtained here for some choice of $\dot{A} = \dot{A}(0)$, then we will say κ is the (relative) condition number of the factor (for this choice of norms). In this case first order (approximate) perturbation bounds can be found by using Taylor series, where if $A + t\Delta A$ has a unique reduction for all $t \in [0, 1]$ and $N + \Delta N$ is the factor corresponding to $A + \Delta A$, then we can show

$$\frac{\|\Delta N\|_\alpha}{\|N\|_\beta} \lesssim \kappa \frac{\|\Delta A\|_\gamma}{\|A\|_\delta},$$

where the notation indicates this is a reliable approximate upper bound only for small enough $\|\Delta A\|_\gamma / \|A\|_\delta$. We will now concentrate mainly on derivative bounds, and say little more about perturbation bounds.

To simplify the presentation we will assume $v_1(t) = v_1$ and $w_1(t) = w_1$ are fixed, so we concentrate in changes in A alone. We will then have $Z_1 = 0$, $Z_0 = Z$ and $M_A = M = V^{-1}\dot{A}V$ in (4.13), see (4.10).

We will use N_L and N_{SL} to denote the lower and strictly lower triangular parts of any matrix N, and N_{SSL} to denote N_{SL} with its next to diagonal elements set to zero, and N_U, N_{SU} and N_{SSU} to denote the upper triangular equivalents.

Because $V = W$ is orthogonal, the case of symmetric $A(t)$ with $v_1(t) = w_1(t)$ in (4.8) has some nice simplifications, so we will treat it first.

6.1. Condition and bounds in the symmetric case

In the symmetric case $W(t) = V(t)$ is orthogonal in (4.9), so $Z = Z_0 = -V^T\dot{V} = \dot{V}^T V$ is skew symmetric and has zero diagonal. Also $M = M_A = V^T \dot{A} V$ is symmetric in (4.10). If we rewrite (4.15) as $Lz = m$, then $\|z\|_2 = \|Z_{SL}\|_F = \|Z_{SU}\|_F = \|Z\|_F/\sqrt{2} = \|\dot{V}\|_F/\sqrt{2}$, $\|m\|_2 = \|M_{SSL}\|_F \le \|M\|_F/\sqrt{2} = \|\dot{A}\|_F/\sqrt{2}$, so since $\|z\|_2 \le \|L^{-1}\|_2 \|m\|_2$,

$$\frac{\|\dot{V}\|_F}{\|V\|_2} = \|\dot{V}\|_F = \|Z\|_F \le \|L^{-1}\|_2 \|\dot{A}\|_F = \|L^{-1}\|_2 \|T\|_2 \frac{\|\dot{A}\|_F}{\|A\|_2}, \tag{6.50}$$

where equality can be obtained for any symmetric A and initial vector v_1 by taking the middle three diagonals of M zero and m to be the right singular vector corresponding to the largest singular value of L^{-1}, and $\dot{A} = VMV^T$. Thus (using 'L' for Lanczos)

$$\kappa_L(A, v_1) \equiv \|L^{-1}\|_2 \|T\|_2 = \|L^{-1}\|_2 \|A\|_2 \tag{6.51}$$

can be thought of as the condition number (for the choice of norms in (6.50)) of V for changes in A in the symmetric Lanczos reduction, that is, for the tridiagonalization of symmetric A by orthogonal similarity transformations with $Ve_1 = v_1$. This special case of symmetric A and $\dot{A}$ for the Lanczos tridiagonalization here corresponds to the same special case for the Arnoldi Hessenberg reduction in [2], and for this case (6.51) corresponds to [2, Thm. 2.(a), p.147]. Note that $\beta_2 = e_2^T T e_1 \le \|T\|_2$ and $\beta_2^{-1} = |e_1^T L^{-1} e_1| \le \|L^{-1}\|_2$, so $\kappa_L(A, v_1) \ge 1$.

Next we use the simple result from (4.13)

$$\|\dot{T}\|_F \le \|M\|_F + 2\|T\|_2\|Z\|_F. \tag{6.52}$$

We see from (4.20), and (4.24)–(4.27), that the elements of $\dot{T}$ depend directly on only those elements of Z in the four diagonals immediately surrounding the main diagonal of Z. But an examination of (4.15) and (5.48) suggest that (6.52) will not give too great an over bound. By using (6.52) we get the weak bound

$$\frac{\|\dot{T}\|_F}{\|T\|_2} \le [1 + 2\kappa_L(A, v_1)]\frac{\|\dot{A}\|_F}{\|A\|_2}. \tag{6.53}$$

6.2. Bounds for the unsymmetric case

Write $Z = [z_1, \dots, z_n]$ *etc.*, with $\bar{Z}$ and Z_D as in Section 4.3.. In the symmetric case $\dot{v}_j = -Vz_j$ is orthogonal to v_j, but in the unsymmetric case this need not be true. Since any change in the direction of v_j leaves us in the subspace of v_j, we will usually only be interested in that part of $\dot{v}_j$ orthogonal to v_j, that is $P_j\dot{v}_j$ with $P_j \equiv I - v_j(v_j^T v_j)^{-1}v_j^T$. Write $\dot{V}_\perp \equiv [P_1\dot{v}_1, \dots, P_n\dot{v}_n]$, then since $P_j\dot{v}_j = -P_jVz_j = -P_jV\bar{z}_j$, we have that $\|P_j\dot{v}_j\|_2 \le \|V\bar{z}_j\|_2$, and so

$$\|\dot{V}_\perp\|_F \le \|V\bar{Z}\|_F \le \|V\|_2\|\bar{Z}\|_F. \tag{6.54}$$

Now we can obtain all our bounds independently of Z_D. From (4.15), (4.17)

$$\|\bar{Z}\|_F^2 = \|Z_{SL}\|_F^2 + \|Z_{SU}\|_F^2 \le \|L^{-1}\|_2^2\|M_{SSL}\|_F^2 + \|U^{-T}\|_2^2\|M_{SSU}\|_F^2.$$

Define $\mu \equiv \max\{\|L^{-1}\|_2, \|U^{-T}\|_2\}$, so

$$\|\bar{Z}\|_F \le \mu\|M\|_F = \mu\|V^{-1}\dot{A}V\|_F,$$

where equality is attainable by choosing $\dot{A}$ carefully. With (6.54) and (4.43) this gives

$$\frac{\|\dot{V}_\perp\|_F}{\|V\|_2} \le \|\bar{Z}\|_F \le \mu\|M\|_F \le \mu\|A\|_2\kappa_2(V)\frac{\|\dot{A}\|_F}{\|A\|_2}, \tag{6.55}$$

$$\frac{\|\dot{T}\|_F}{\|T\|_2} \le (1 + 2\mu\|T\|_2)\frac{\|M\|_F}{\|T\|_2}, \tag{6.56}$$

so $\max\{\|L^{-1}\|_2, \|U^{-T}\|_2\}\|A\|_2\kappa_2(V)$ might be a reasonable (bound on the) condition number for changes in V. Unfortunately with the *a priori* bounds

$$\kappa_2(V)^{-2}\frac{\|\dot{A}\|_F}{\|A\|_2} \le \frac{\|M\|_F}{\|T\|_2} = \frac{\|V^{-1}\dot{A}V\|_F}{\|V^{-1}AV\|_2} \le \kappa_2(V)^2\frac{\|\dot{A}\|_F}{\|A\|_2},$$

(6.56) gives an apparently weak bound in the general case, but (6.55) and (6.56) become (6.50) and (6.53) in the symmetric case.

6.3. Partial reductions

In many applications we are interested in the sensitivities for $k < n$ steps of the Lanczos reduction. The notation is messy, so we treat this separately. When we deal with $n \times n$ matrices, N_{ij} will for example denote the leading principle $i \times j$ submatrix of N, but for a fixed k we will mix this standard notation with the following. Single superscripts (1) and (2) will denote column partitions as in $V = [V^{(1)}, V^{(2)}]$, $V^{(1)}$ having k columns, and double superscripts (12) *etc.* will denote block partitions:

$$Z = [Z^{(1)}, Z^{(2)}] = \begin{pmatrix} Z^{(11)} & Z^{(12)} \\ Z^{(21)} & Z^{(22)} \end{pmatrix}, \qquad Z^{(11)} \quad k \times k.$$

For the higher dimensional matrices L and U in (4.15)–(4.16) and (4.17)–(4.18), $L^{(11)}$ *etc.* will denote the leading principal $(k-1)$-block by $(k-1)$-block submatrix.
The initial $k \times k$ submatrix of (4.43) then gives

$$\dot{T}_{kk} = \tfrac{1}{2}(D_{kk}N_{kk}^T D_{kk}^{-1} + N_{kk}), \quad N_{kk} = M_{kk} + \bar{Z}_{k,k+1}T_{k+1,k} - T_{k,k+1}\bar{Z}_{k+1,k}, \quad (6.57)$$

so a bound on $\dot{T}_{kk}$ requires knowledge of $\bar{Z}_{k+1,k+1}$. Because $\bar{Z}$ has zero diagonal, this only requires knowledge of the first k columns and rows of $\bar{Z}$. But from (4.15) and (4.17) with $L^{(11)}$ and $U^{(11)}$ as above,

$$\begin{aligned} L^{(11)} \begin{pmatrix} z_{3:n,2} \\ \cdot \\ z_{k+1:n,k} \end{pmatrix} &= \begin{pmatrix} m_{3:n,1} \\ \cdot \\ m_{k+1:n,k-1} \end{pmatrix} \equiv m \quad \text{say}, \qquad (6.58) \\ U^{(11)T} \begin{pmatrix} z_{2,3:n}^T \\ \cdot \\ z_{k,k+1:n}^T \end{pmatrix} &= \begin{pmatrix} m_{1,3:n}^T \\ \cdot \\ m_{k-1,k+1:n}^T \end{pmatrix}, \end{aligned}$$

so with $Z_{SL}^{(1)}$ denoting the first k columns of Z_{SL} *etc.*, equality is attainable simultaneously in the following by choosing M correctly:

$$\begin{aligned} \|Z_{SL}^{(1)}\|_F &\leq \|L^{(11)-1}\|_2 \|(M_{SSL})_{k-1}\|_F, \\ \|(Z_{SU}^T)^{(1)}\|_F &\leq \|U^{(11)-1}\|_2 \|(M_{SSU}^T)_{k-1}\|_F. \end{aligned}$$

Now $L^{(11)-1}$ and $U^{(11)-T}$ are the leading principal $(k-1)$-block by $(k-1)$-block submatrices of L^{-1} and U^{-T}, whose subblocks are given in (5.48) and (5.49). Let $\hat{E}$ be the matrix obtained by deleting rows $k+1:n$ of every block-row of $L^{(11)-1}$, $\bar{E}$ the matrix obtained by retaining just those rows, and $\tilde{E}$ be the matrix obtained by deleting rows $k+2:n$ of every block-row of $L^{(11)-1}$ (so from (6.58) $\hat{E}m$ gives the unknown elements of $Z_{SL}^{(11)}$, $\bar{E}m$ gives the unknown elements of $Z_{SL}^{(21)}$, and $\tilde{E}m$ gives the unknown elements of $(Z_{SL})_{k+1,k+1}$), and let $\hat{F}$, $\bar{F}$ and $\tilde{F}$ be the equivalent matrices for $U^{(11)-T}$, then

$$\begin{aligned} \|Z_{SL}^{(11)}\|_F \leq \|\hat{E}\|_2 \|(M_{SSL})_{k-1}\|_F, \qquad & \|Z_{SU}^{(11)}\|_F \leq \|\hat{F}\|_2 \|(M_{SSU}^T)_{k-1}\|_F, \\ \|Z_{SL}^{(21)}\|_F \leq \|\bar{E}\|_2 \|(M_{SSL})_{k-1}\|_F, \qquad & \|Z_{SU}^{(12)}\|_F \leq \|\bar{F}\|_2 \|(M_{SSU}^T)_{k-1}\|_F, \\ \|(Z_{SL})_{k+1,k+1}\|_F \leq & \|\tilde{E}\|_2 \|(M_{SSL})_{k-1}\|_F, \end{aligned}$$

$$\|(Z_{SU})_{k+1,k+1}\|_F \quad \le \quad \|\tilde{F}\|_2\|(M_{SSU}^T)_{k-1}\|_F.$$

Now let $\mu_k \equiv \max\{\|L^{(11)-1}\|_2, \|U^{(11)-1}\|_2\}$, $\hat{\mu}_k \equiv \max\{\|\hat{E}\|_2, \|\hat{F}\|_2\}$, $\bar{\mu}_k \equiv \max\{\|\bar{E}\|_2, \|\bar{F}\|_2\}$ and $\tilde{\mu}_k \equiv \max\{\|\tilde{E}\|_2, \|\tilde{F}\|_2\}$, then we see

$$\begin{array}{rcl} \hat{\mu}_k \le \tilde{\mu}_k \le \mu_k, & & \bar{\mu}_k \le \mu_k, \qquad \mu_k^2 \le \hat{\mu}_k^2 + \bar{\mu}_k^2, \\ \|\bar{Z}^{(1)}\|_F^2 & = & \|Z_{SL}^{(1)}\|_F^2 + \|Z_{SU}^{(11)}\|_F^2 \\ & \le & \|L^{(11)-1}\|_2^2\|(M_{SSL})_{k-1}\|_F^2 + \|\hat{F}\|_2^2\|(M_{SSU}^T)_{k-1}\|_F^2 \\ & \le & \mu_k^2\|M\|_F^2, \\ \|\bar{Z}^{(11)}\|_F & \le & \hat{\mu}_k\|M\|_F, \\ \|Z^{(21)}\|_F & = & \|\bar{Z}^{(21)}\|_F = \|Z_{SL}^{(21)}\|_F \le \bar{\mu}_k\|M\|_F, \\ \|\bar{Z}_{k+1,k+1}\|_F & \le & \tilde{\mu}_k\|M\|_F, \end{array}$$

where these can be loose because we replaced the first $k-1$ columns and rows of M, less its main tridiagonal, by M. Next since

$$\begin{array}{rcl} \|\bar{Z}_{k,k+1}\|_F, \|\bar{Z}_{k+1,k}\|_F & \le & \|\bar{Z}_{k+1,k+1}\|_F, \\ \|T_{k+1,k}\|_2, \|T_{k,k+1}\|_2 & \le & \|T_{k+1,k+1}\|_2, \end{array}$$

we see from (6.57)

$$\begin{array}{rcl} \|\dot{T}_{kk}\|_F & \le & \|M_{kk}\|_F + 2\|T_{k+1,k+1}\|_2\|\bar{Z}_{k+1,k+1}\|_F \\ & \le & (1 + 2\tilde{\mu}_k\|T_{k+1,k+1}\|_2)\|M\|_F \le (1 + 2\tilde{\mu}_k\|T\|_2)\|M\|_F, \end{array}$$

which is similar in form to (6.56).

For the first k columns of $\dot{V}_\perp$ in (6.54) we have, similar to (6.55),

$$\|\dot{V}_\perp^{(1)}\|_F \le \|V\bar{Z}^{(1)}\|_F \le \|V\|_2\mu_k\|M\|_F \le \|V\|_2\mu_k\kappa_2(V)\|\dot{A}\|_F,$$

so $\max\{\|L^{(11)-1}\|_2, \|U^{(11)-1}\|_2\}\|A\|_2\kappa_2(V)$ might be a reasonable (bound on the) condition number for changes in $V^{(1)}$.

6.3.1. Krylov subspaces. Since $V = V(0)$ is nonsingular and $V(t)$ in (4.9) is differentiable for small enough t, it has a unique QR factorization

$$V(t) = Q(t)R(t), \qquad Q(t)^TQ(t) = I, \qquad R(t) \ \text{ upper triangular},$$

when we take the diagonal of $R(t)$ positive. Then it can be seen from examining the algorithm for the QR factorization, see for example [9], that $Q(t)$ and $R(t)$ are differentiable for small enough t.

Write $Q \equiv Q(0)$, $R \equiv R(0)$, and partition the matrices as in

$$\begin{array}{l} V(t) = [V^{(1)}(t), V^{(2)}(t)], \\ Q(t) = [Q^{(1)}(t), Q^{(2)}(t)], \end{array} \qquad R(t) = \begin{bmatrix} R^{(11)}(t) & R^{(12)}(t) \\ 0 & R^{(22)}(t) \end{bmatrix},$$

where $V^{(1)}(t)$ and $Q^{(1)}(t)$ are $n \times k$ and $R^{(11)}(t)$ is $k \times k$, then we have $V^{(1)}(t) = Q^{(1)}(t)R^{(11)}(t)$, and $\mathcal{R}(V^{(1)}(t)) = \mathcal{R}(Q^{(1)}(t))$ is the Krylov subspace formed by

k steps of the Lanczos algorithm with $A(t)$ and starting vectors $v_1(t)$ and $w_1(t)$. For small t we are interested in the distance between this and the original Krylov subspace $\mathcal{R}(V^{(1)}) = \mathcal{R}(Q^{(1)})$. It was shown in [4] that the sines of the angles between $\mathcal{R}(Q^{(1)})$ and $\mathcal{R}(Q^{(1)}(t))$ are the singular values of $Q^{(2)T}Q^{(1)}(t)$ (the cosines are the singular values of $Q^{(1)T}Q^{(1)}(t)$). It follows that one simple overall measure of the distance between the subspaces $\mathcal{R}(V^{(1)}(t))$ and $\mathcal{R}(V^{(1)})$ is $\|Q^{(2)T}Q^{(1)}(t)\|_F$, the square root of the sum of squares of these sines, and we will use this.

But if $\kappa_{KS}(A, v_1, w_1, k)$ is such that, writing $\dot{Q} \equiv \dot{Q}(0)$,

$$\|Q^{(2)T}\dot{Q}^{(1)}\|_F \leq \kappa_{KS}(A, v_1, w_1, k)\frac{\|\dot{A}\|_F}{\|A\|_2}$$

with equality attainable for any A by choosing $\dot{A}$ correctly, then we can show for small enough ΔA in $A(t) = A + t\Delta A$ that we have the first order bound

$$\|Q^{(2)T}Q^{(1)}(1)\|_F \lesssim \kappa_{KS}(A, v_1, w_1, k)\frac{\|\Delta A\|_F}{\|A\|_2}$$

on the distance between the subspaces $\mathcal{R}(V^{(1)}(1))$ and $\mathcal{R}(V^{(1)})$. As a result the condition number for the Krylov subspace $\mathcal{R}(V^{(1)})$ is $\kappa_{KS}(A, v_1, w_1, k)$, for this choice of norms. We will now show how to at least bound this.

Writing $\dot{V}^{(1)} = \dot{V}^{(1)}(0)$, we see with (4.12) $V^{(1)}(t) = Q^{(1)}(t)R^{(11)}(t)$ gives

$$\begin{aligned} \dot{V}^{(1)} &= \dot{Q}^{(1)}R^{(11)} + Q^{(1)}\dot{R}^{(11)} = -VZ^{(1)} = -QRZ^{(1)}, \\ Q^{(2)T}\dot{V}^{(1)} &= Q^{(2)T}\dot{Q}^{(1)}R^{(11)} = -Q^{(2)T}QRZ^{(1)} = -R^{(22)}Z^{(21)}, \end{aligned}$$

and noting $\bar{Z}^{(21)} = Z^{(21)}$ we see

$$\begin{aligned} \|Q^{(2)T}\dot{Q}^{(1)}\|_F &= \|R^{(22)}Z^{(21)}R^{(11)-1}\|_F \leq \|R^{(22)}\|_2\|R^{(11)-1}\|_2\|Z^{(21)}\|_F \\ &\leq \bar{\mu}_k\|R^{(22)}\|_2\|R^{(11)-1}\|_2\|M\|_F \\ &\leq \bar{\mu}_k\kappa_2(V)\|R^{(22)}\|_2\|R^{(11)-1}\|_2\|\dot{A}\|_F. \qquad (6.59) \end{aligned}$$

Thus $\nu_{KS}(A, v_1, w_1, k) \equiv \bar{\mu}_k\kappa_2(V)\|A\|_2\|R^{(22)}\|_2\|R^{(11)-1}\|_2$ gives an upper bound on $\kappa_{KS}(A, v_1, w_1, k)$, but a more careful analysis should give a better bound. When A and $\dot{A}$ are symmetric, we see $\nu_{KS}(A, v_1, v_1, k) = \bar{\mu}_k\|A\|_2$, and in this case it can be seen the bound (6.59) is attainable, so $\bar{\mu}_k\|A\|_2$ is the required condition number for the the Krylov subspace $\mathcal{R}(V^{(1)})$. For this special symmetric case this corresponds to [2, Thm. 2.(b), p.147].

6.4. Estimating condition numbers

Since the lower triangular matrix L in (4.16) (or U^T) has $O(n^2)$ elements (about $5n^2/2$), $\|L^{-1}\|_2$ and the condition numbers and bounds here, see for example (6.51), could be adequately estimated in $O(n^2)$ floating point operations, see Higham [11,12], where of course L would never be formed, the estimates being obtained from T alone. However even $O(n^2)$ is large for large n, and in that case some cheaper method of estimation could be desirable, perhaps one based on the expressions for the inverses L^{-1} and U^{-T} in Section 5.. In the partial reduction case we are only looking at $O(kn)$ elements in the triangular matrices. However in both cases it appears important to use the knowledge of the inverses in Section 5. to obtain better approximations to the condition numbers in the unsymmetric case, and numerical bounds for these approximations.

7. Conclusions and comparisons with related work

For the Lanczos reduction (1.1)–(1.2), we considered how the choice of normalization affects the sensitivity of the problem. We then showed that by defining

$$Z_0 \equiv -V^{-1}\dot{V}, \qquad M_A \equiv V^{-1}\dot{A}V$$

in (4.10), we split the sensitivity analysis of the reduction into subproblems. This gave the lower triangular system (4.15)–(4.16) for the elements of the strictly lower triangle of Z, the unknown part of Z_0, and the lower triangular system (4.17)–(4.18) for the elements of the strictly upper triangle of Z. These systems could be solved independently of each other, the diagonal of Z, and the elements of $\dot{T}$. We saw that all the sensitivities of interest then depended directly on these off-diagonal elements of Z.

The off-diagonal elements of Z depend on the elements of M_A above, see (4.13) and (4.15), and so ill-conditioned V can cause large sensitivity. This effect is absent when A is symmetric or nearly so resulting in V being orthogonal or nearly so.

The strictly lower triangle of Z is the solution of (4.15), where from (5.48) the (i, j)-th block of L^{-1} involves the multiplicative factor $(\beta_{j+1} \cdots \beta_{i+1})^{-1}$. Similarly the strictly upper triangle of Z is the solution of (4.17), where from (5.49) the (i, j)-th block of U^{-T} involves the multiplicative factor $(\gamma_{j+1} \cdots \gamma_{i+1})^{-1}$. This suggests how one small, or a few fairly small, next to diagonal elements of T can contribute to the sensitivity of the reduction.

Theorem 4.1. gave a full description of the sensitivities, while Section 5. gave the inverses of the matrices involved. Section 6. applied some of these results in showing how some condition numbers and bounds could be obtained. It dealt briefly with the symmetric and unsymmetric cases, and the full and partial factors, and in this last case considered the sensitivity of the Krylov subspaces. The bounds obtained in all the unsymmetric cases look weak, and can hopefully be improved.

A related problem to the sensitivity analysis of the symmetric case was studied by Le and Parlett [15]. There they looked at the forward stability of the QR algorithm with shifts, where one step results in a new symmetric tridiagonal $\hat{T} = Q^T T Q$, Q orthogonal. They showed that forward instability occurs only when the shift is very close to certain eigenvalues. The ideas of forward instability of such a backward stable algorithm are closely related to sensitivity analysis, in that the computed result is exact for nearby data, so their result could also be proven from the work here if we could show that the reduction is sensitive only when the shift is very close to certain eigenvalues. A possible approach would be to show, using (5.48), that some block X_{ij} of L^{-1} in (6.51) can be large only when the shift is very close to certain eigenvalues. The fact that a shift that is *equal* to an eigenvalue will lead to a zero next to diagonal element suggests such a proof might be possible.

Carpraux, Godunov and Kuznetsov [2] studied a closely related problem to the one here: the sensitivity of Krylov subspaces $\mathcal{K}_k(A, v_1) = \mathrm{span}\{v_1, Av_1, .., A^{k-1}v_1\}$, $k = 1, \ldots, n$, and of the corresponding *orthogonal* Krylov bases. Note that our bases $\{v_1, \ldots, v_k\}$ in (4.29) are only orthogonal in the symmetric case, but that $\mathcal{K}_k(A, v_1) = \mathrm{span}\{v_1, \ldots, v_k\}$, so, using a different approach, we have studied the sensitivities of the same Krylov *subspaces* as in [2]. Carpraux *et al.* showed how the condition in the general case could be expressed in terms of the inverse of a large triangular matrix formed from the elements of upper Hessenberg P^TAP with P orthogonal.

In particular they developed the subspace and orthogonal basis condition numbers for $k = 1, \ldots, n$, but did not consider the sensitivity of the Arnoldi Hessenberg reduction [1]. On the other hand we considered the sensitivity of the Lanczos tridiagonal reduction, both full and partial, and gave bounds on the condition numbers for the nonorthogonal bases (partial factors $[v_1, \ldots, v_k]$) and the Krylov subspaces for $k = 1, \ldots, n$. In the symmetric case where these two approaches overlap we found corresponding condition numbers to those in [2] (identical if we replace their $\|A\|_F$ by our $\|A\|_2$), but because we were dealing with nonorthogonal bases, and did not have the time to develop tight bounds, we apparently only produced upper bounds in the unsymmetric case, not actual condition numbers.

The Krylov subspace and biorthogonal basis sensitivity results from the Lanczos algorithm are available here for use with methods based on the Lanczos algorithm, since the T would be available — while the Krylov subspace and orthogonal basis sensitivity results in [2] are available for use with methods based on the Arnoldi algorithm [1], since those produce the required Hessenberg matrix.

An advantage of the approach here is that for the Lanczos reduction we gave a very simple and direct derivation of the linear system expressing the sensitivity, and showed how the inverse of our large triangular matrix could be expressed in terms of polynomials, see (5.48). In fact in the symmetric case the Hessenberg matrix in [2] becomes our T in (1.2), and then the lower triangular matrix in [2, p. 151] becomes $-L^{(11)}$ in (6.58), the leading $k-1$ block by $k-1$ block of $-L$ in (4.16), and so the two somewhat different approaches to these two related problems result in the identical expression in the common case.

This paper needs to be extended in several obvious ways. Use needs to be made here of the known form of the inverses in Section 5. in order to derive superior condition estimates. The unsymmetric case here needs to be examined more closely to see if for some choice of norms condition *numbers* can be obtained, rather than the upper bounds derived here. Finally the approach used here could perhaps be applied to the problem in [2], to see if their important results could be derived a bit more simply.

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