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ON THE ERROR IN THE PRODUCT QR DECOMPOSITION*

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Abstract. We develop both a normwise and a componentwise error analysis for the QR factorization of long products of invertible matrices. We obtain global error bounds for both the orthogonal and upper triangular factors that depend on uniform bounds on the size of the local error, the local degree of nonnormality, and integral separation, a natural condition related to gaps between eigenvalues but for products of matrices. We illustrate our analytical results with numerical results that show the dependence on the degree of nonnormality and the strength of integral separation.

Key words. QR decomposition, matrix product, integral separation

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1. Introduction.

In this paper we consider perturbation analysis for the QR decomposition of long products of matrices. In particular, we obtain uniform norm bounds and componentwise bounds on the orthogonal and upper triangular factors under the assumption of integral separation. Integral separation is a natural analogue for products of matrices to having gaps between eigenvalues of a matrix. Our approach is based upon ideas that are central to perturbation theory for Lyapunov exponents of linear nonautonomous differential equations. In particular, the results obtained here improve upon the results that can be obtained by combining the results in [8] and [11] by requiring less stringent assumptions and by obtaining sharper bounds. Here we avoid an intermediate step in which a perturbed triangular differential equation is obtained and work directly with perturbed triangular matrix products.

We consider sources of perturbation error that include roundoff error, measurement error, and discretization error due, for example, to approximating the solution of a differential equation. The difficulty or conditioning of the problem is characterized by the degree of nonnormality and the strength of integral separation. The results we obtain allow for error bounds up to a certain size and structure in the perturbation error as compared with the conditioning of the problem.

Our work here draws motivation from the work on QR and singular value decompositions of long matrix products (see, e.g., [22, 20, 18, 14, 15]) as well as the perturbation results for the QR factorization of a matrix, for example, [21, 23, 24, 5, 6]. We make use of the structural assumption of integral separation, which is central to the perturbation theory for Lyapunov exponents, stability spectra that play an analogous role to the real parts of eigenvalues for nonautonomous linear differential equations. An excellent reference that summarizes many results on Lyapunov exponents is the monograph by Adrianova [1]. In a series of papers [7, 8, 9, 10, 11], Dieci and the author have justified and developed an error analysis for approximation of Lyapunov exponents for nonautonomous linear differential equations via continuous QR factorizations of fundamental matrix solutions.

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This paper is organized as follows. In section 2 we re-create an argument that shows how the product QR algorithm applied to a sequence of perturbed and unperturbed invertible matrices reduces the error analysis to perturbed and unperturbed invertible triangular matrices. In section 3 we formulate the problem of determining global error bounds as a zero finding problem, present the Newton–Kantorovich-type theorem we will employ, and provide background on our main structural assumption, integral separation. Our main results on obtaining norm bounds are stated and subsequently proved in section 4. Since the zero finding problem as formulated is quadratic, the second derivative is constant which simplifies the analysis. In section 5 we extend the results to componentwise bounds by employing a simple change of variables and a weighted norm and show how the assumption of integral separation can be relaxed. We present numerical results in section 6 to illustrate the efficacy of our analysis, and in section 7 we summarize and state some conclusions and avenues for future research.

2. Background. Consider determining an orthogonal change of variables that brings the linear discrete time varying problem (A_n an $m \times m$ invertible matrix with real entries for all n),

$$x_{n+1} = A_n x_n, \;\; n = 0, 1, \dots,$$

to upper triangular form; i.e., given $\tilde{Q}_0$ orthogonal, determine a sequence of orthogonal matrices, $\{\tilde{Q}_k\}_{k=1}^{\infty}$, and a sequence of upper triangular matrices with positive diagonal elements, $\{\tilde{R}_k\}_{k=0}^{\infty}$, such that

$$\tilde{Q}_{n+1}\tilde{R}_n = A_n \tilde{Q}_n, \;\; v_{n+1} = \tilde{R}_n v_n, \;\; x_n = \tilde{Q}_n v_n, \tag{2.1}$$

for example, by applying the (modified) Gram–Schmidt procedure to $A_n\tilde{Q}_n$. Thus,

$$A_k \cdots A_0 \tilde{Q}_0 = \tilde{Q}_{k+1}\tilde{R}_k \cdots \tilde{R}_0.$$

In addition, consider the perturbed problem

$$y_{n+1} = [A_n + F_n] y_n, \;\; n = 0, 1, \dots,$$

with $A_n + F_n$ invertible for all n (for example, if $\|F_n\|_2 < \sigma_{min}(A_n)$, the smallest singular value of A_n) which may be transformed to upper triangular form

$$\overline{Q}_{n+1} R_n = [A_n + F_n]\overline{Q}_n, \;\; w_{n+1} = R_n w_n, \;\; y_n = \overline{Q}_n w_n, \tag{2.2}$$

where the $\overline{Q}_n$ are orthogonal and the R_n are upper triangular with positive diagonal elements. We are using $\tilde{Q}_n$ and $\tilde{R}_n$ as the exact orthogonal and upper triangular matrices, respectively, and $\overline{Q}_n$ and R_n as the perturbed or approximate orthgonal and upper triangular matrices, respectively.

Following Theorem 3.1 of [8], we note that if $\tilde{Q}_0 = \overline{Q}_0$, then

$$\tilde{Q}_{k+1}\tilde{R}_k \cdots \tilde{R}_0 = \overline{Q}_{k+1}[R_k + E_k] \cdots [R_0 + E_0], \tag{2.3}$$

where $E_j = -\overline{Q}_{j+1}^T F_j \overline{Q}_j$. Thus, if $[R_k + E_k] \cdots [R_0 + E_0] = Q_{k+1} U_k$ for some orthogonal Q_{k+1} and upper triangular U_k (with positive diagonal elements), then by uniqueness of the QR factorization of an invertible matrix

$$\tilde{Q}_{k+1} = \overline{Q}_{k+1} Q_{k+1}, \;\; \|\overline{Q}_{k+1} - \tilde{Q}_{k+1}\| = \|I - Q_{k+1}\|,$$

so the global error is small if the sequence of Q_k's is uniformly near the identity. The error matrices E_j's are functions of the computed $\overline{Q}_j$'s and the original error matrices, the F_j's. Thus, any information about the F_j that is known can be used to determine the form of the error term E_j.

Remark 2.1. We note that the process described in (2.1) is essentially orthogonal or QR iteration [12] when $A_n \equiv A$ for all n. On the other hand, a shifted QR iteration may be interpreted in terms of a sequence of matrices $\{A_k\}_{k=0}^{\infty}$.

3. Formulation.

We formulate the problem of showing the existence of a near identity orthogonal change of variables for the sequence of perturbed upper triangular matrices, $R_n + E_n$, as one of finding a solution to a functional equation $G(\{Q_k\}_{k=1}^{\infty}) = 0$, where for $n = 0, 1, \dots$ the nth element of G is given by two components,

$$(G(\{Q_k\}_{k=1}^{\infty}))_n = \begin{pmatrix} (G_1(\{Q_k\}_{k=1}^{\infty}))_n \\ (G_2(\{Q_k\}_{k=1}^{\infty}))_n \end{pmatrix}, \tag{3.1}$$

where $Q_0 = I$ and

$$\begin{aligned} (G_1(\{Q_k\}_{k=1}^{\infty}))_n &= \mathtt{slow}(Q_{n+1}^T[R_n + E_n]Q_n) \\ (G_2(\{Q_k\}_{k=1}^{\infty}))_n &= \mathtt{upp}(Q_{n+1}Q_{n+1}^T - I), \end{aligned} \tag{3.2}$$

where `slow` denotes the strictly lower triangular part of a matrix and `upp` the upper triangular part. Similarly, we will employ `low`, the lower triangular part of a matrix, and `supp`, the strictly upper triangular part of a matrix. In (3.2) G_1 being zero ensures that the $Q_{n+1}^T[R_n + E_n]Q_n$ is upper triangular for all n, while G_2 being zero ensures that the Q_n's are orthogonal.

3.1. Convergence of a Newton iteration.

To obtain error bounds we will employ the following convergence result for Newton's method with perturbed Jacobian applied to the $G(\{Q_k\}_{k=1}^{\infty}) = 0$ with initial guess $\{Q_k^{(0)}\}_{k=1}^{\infty}$, where $Q_k^{(0)} = I$ for all k. The problem of showing convergence of a Newton iteration is somewhat simplified for (3.1) and (3.2) since the problem is naturally quadratic and hence second derivative bounds in a neigborhood needed to prove the convergence of a Newton iteration may be evaluated at an arbitrary point. Our main result involves employing Theorem 1 of [13, p. 536] which we summarize below. The following theorem applies when there exists a sufficiently good invertible approximation Γ to $G'(x_0)$, where x_0 is the initial guess for the Newton-like iteration. The theorem may be applied in a general Banach space setting. In what follows we will initially employ a norm of the form $\|V\| = \sup_n \|V_n\|_F$, where $V = \{V_n\}_{n=1}^{\infty}$, for matrices V_n to obtain norm bounds and subsequently a weighted supremum norm to obtain componentwise bounds.

THEOREM 3.1. *Suppose there exists a linear operator Γ having continuous inverse and the following conditions are satisfied:*

$$\|\Gamma^{-1}G(x_0)\| \le \eta, \tag{3.3}$$

$$\|\Gamma^{-1}G'(x_0) - I\| \le \delta, \tag{3.4}$$

and

$$\|\Gamma^{-1}G''(x)\| \le K \ \ \forall x \in \Omega_0, \tag{3.5}$$

where Ω_0 is a sufficiently large neighborhood of x_0. If $\delta < 1$ and $h := \frac{\eta K}{(1-\delta)^2} < \frac{1}{2}$, then there exists a solution x^* of $G(x) = 0$ such that $\|x^* - x_0\| \le r_0$, where $r_0 = (1 - \sqrt{1-2h})(1-\delta)/K \equiv 2\eta/(1-\delta)(1+\sqrt{1-2h})$.

This theorem provides a bound r_0 on the difference between the initial guess, x_0, and the x^* such that $G(x^*) = 0$, provided $h < 1/2$. For the problem we consider, $G(\{Q_k\}_{k=1}^{\infty}) = 0$ for G defined in (3.1) and (3.2), we have the $Q_k = I$ for all k is a solution when the error $E_k \equiv 0$ for all k. Thus, for $\|E_k\|$ uniformly small enough in k, one might expect a solution $Q_k \approx I$.

3.2. Integral separation. A natural assumption that will ensure the existence of a solution, a near identity orthogonal change of variables, given a small enough error is integral separation.

DEFINITION 3.2. *Two positive sequences* $\{\alpha_k\}_{k=0}^{\infty}$ *and* $\{\beta_k\}_{k=0}^{\infty}$ *are* integrally separated *if there exists constants* $\Omega,\ \lambda$ *with* $0 < \Omega \leq 1$ *and* $\lambda > 1$ *such that for* $t \geq s$,

$$\prod_{k=s}^{t} \frac{\alpha_k}{\beta_k} \geq \Omega \lambda^{(t-s)}.$$

Assumption. We assume that the diagonal elements of the R_n are integrally separated, i.e., for $i > j$ there exists $\Omega_{ij}, \lambda_{ij}$ with $0 < \Omega_{ij} \leq 1$ and $\lambda_{ij} > 1$ such that for $t \geq s$,

$$\prod_{k=s}^{t} \frac{(R_k)_{jj}}{(R_k)_{ii}} \geq \Omega_{ij} \lambda_{ij}^{(t-s)}. \tag{3.6}$$

Integral separation plays the role of gaps between eigenvalues in the case of a sequence of possibly different matrices. It will imply a conditional contractivity property for a Newton-type mapping applied to (3.1) and (3.2) that will be analyzed in the next section. In the case in which $A_n \equiv A$ for a single invertible matrix A, the system is integrally separated provided the real parts of the eigenvalues of A are distinct. It is possible to obtain perturbation results in the nonintegrally separated case, for example, for A with a complex conjugate pair of eigenvalues; see, for example, section 4 of [9].

An important consequence of this assumption is that for $i > j$,

$$\sum_{l=1}^{n} \prod_{k=l}^{n} \frac{(R_k)_{ii}}{(R_k)_{jj}} \leq \left[\frac{1}{\Omega_{ij}}(1 + \lambda_{ij}^{-1} + \cdots \lambda_{ij}^{-n+1})\right] \leq \left[\frac{\lambda_{ij}}{\Omega_{ij}(\lambda_{ij} - 1)}\right] =: \Lambda_{ij} - 1. \tag{3.7}$$

Remark 3.1. The assumption of integral separation is very natural for two important reasons. For continuous time problems, Palmer [19, p. 21] and Millionshchikov [17] showed that in the Banach space $\mathcal{B}$ of continuous bounded matrix valued functions A, with norm $||A|| = \sup_{t\geq 0} ||A(t)||$, that the systems with integral separation form an open and dense subset of $\mathcal{B}$. Thus, integral separation is a generic property in $\mathcal{B}$. In addition, if the Lyapunov exponents, which for triangular systems of the form (2.1) are defined as

$$\lambda_i = \limsup_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} \log((R_k)_{ii}),$$

are distinct, then (see [1]) they are continuous with respect to perturbations in the coefficient matrix function if and only if the system is integrally separated. Similar results should hold in the discrete time setting and are immediate when a continuous time system with piecewise constant coefficient matrix function may be formed through logarithms of the matrices in the discrete time system.

4. Results. We next state our main result whose proof relies on estimates that are shown in the remainder of the section.

THEOREM 4.1. *There exists a sequence of orthogonal matrices* $\{Q_k\}_{k=0}^{\infty}$ *with* $Q_0 = I$ *such that*

$$Q_{n+1}\overline{R}_n = [R_n + E_n]Q_n, \quad n = 0, 1, \dots, \tag{4.1}$$

provided $R_n + E_n$ *is invertible for all* n *where* R_n *and* $\overline{R}_n$ *are upper triangular with positive diagonal elements. Moreover, if* (3.6) *holds, then there exists an invertible operator* Γ *such that the corresponding* η, δ, K *in Theorem* 3.1 *have the bounds for* Λ_{ij} *defined in* (3.7),

$$\eta = \sqrt{2}\left(\sum_{j=1}^{m-1}\sum_{i=j+1}^{m}\left(\Lambda_{ij}\frac{|E_{ij}|}{R_{jj}}\right)^2\right)^{1/2}, \tag{4.2}$$

where $|E_{ij}|/R_{jj} = \sup_n |(E_n)_{ij}|/(R_n)_{jj}$,

$$\delta = \sqrt{2}\left(\sum_{j=1}^{m-1}\sum_{i=j+1}^{m}\left(\Lambda_{ij}\frac{|W_{ij}|}{R_{jj}}\right)^2\right)^{1/2} \tag{4.3}$$

where $\frac{|W_{ij}|}{R_{jj}}$ *is defined as in* (4.17) *below, and*

(4.4)
$$\frac{|W_{ij}|}{R_{jj}} \le \sup_n\, (R_n)_{jj}^{-1}\left[\|(E_n)_{\cdot j}\|_2 + \|(E_n)_{i\cdot}\|_2 + \left(\sum_{k=1}^{j-1}(R_n)_{kj}^2\right)^{1/2} + \left(\sum_{k=i+1}^{m}(R_n)_{ik}^2\right)^{1/2}\right],$$

and

$$K = \left(1 + \sum_{j=1}^{m-1}\sum_{i=j+1}^{m}\Lambda_{ij}^2(|\tilde{W}_{ij}|^2 + |\overline{W}_{ij}|^2)\right)^{1/2}, \tag{4.5}$$

where $|\tilde{W}_{ij}|$ *and* $|\overline{W}_{ij}|$ *are defined as in* (4.25) *and* (4.26), *respectively, and*

$$\begin{aligned} |\tilde{W}_{ij}| &\le \sup_n \frac{1}{(R_n)_{jj}} + 2(\|R_n^{(jj)}\|_F + \|E_n^{(jj)}\|_F) \text{ and} \\ |\overline{W}_{ij}| &\le \sup_n 2(\|R_n^{(jj)}\|_F + \|E_n^{(jj)}\|_F) + 1, \end{aligned} \tag{4.6}$$

$R_n^{(jj)} = (R_n)_{jj}^{-1}R_n$ *and* $E_n^{(jj)} = (R_n)_{jj}^{-1}E_n$. *If* $\delta < 1$ *and* $h := \frac{\eta K}{(1-\delta)^2} < \frac{1}{2}$, *then the conclusion of Theorem* 3.1 *holds and*

$$\sup_n \|Q_n - I\|_F \le r_0 \equiv \frac{2\eta}{(1-\delta)(1+\sqrt{1-2h})}. \tag{4.7}$$

Moreover, for all n, *by uniqueness* $\overline{R}_n = \tilde{R}_n$, *the exact local upper triangular factor in* (2.1), *and*

$$\|\overline{R}_n - R_n\|_F \le 2r_0\|R_n\|_F + \|E_n\|_F. \tag{4.8}$$

Proof. The proof of existence follows from the invertibility of the $R_n + E_n$. The proof of (4.7) is an application of the Newton–Kantorovich theorem (Theorem 3.1) with the initial guess $x_0 \equiv \{Q_k^{(0)}\}_{k=1}^\infty = \{I\}_{k=1}^\infty$, $Q_0 = I$, and the estimates that follow in a series of lemmas (Lemma 4.2 for the bound η, Lemma 4.3 for the bound δ, and Lemma 4.4 for the bound K), while the bound (4.8) is obtained using (4.1) from (4.7) by the triangle inequality. ▯

Remark 4.1. The bound $h < 1/2$ may be satisfied when $\delta < 1$ for $\|E_j\|$ sufficiently small. Having $\delta < 1$ relies upon the strength of the integral separation and the difference between the exact and the perturbed Jacobian. For example, for an integrally separated problem, $\delta < 1$ provided the R_j are sufficiently close to diagonal and the $\|E_j\|$ are sufficiently small. To obtain improved bounds, the bounds in terms of integral separation constants Λ_{ij} may be replaced with bounds in terms of the actual diagonal elements of R, i.e., for $i > j$, $1 + \sum_{l=1}^n \prod_{k=l}^n \frac{(R_k)_{ii}}{(R_k)_{jj}}$ instead of the bound in (3.7).

The analysis here improves upon the techniques developed in [9] and [11] in some important ways. The previous analysis was for nonautonomous differential equations in which the sequence of matrices, the A_n, were transition fundamental matrices. The starting point in [9] was a perturbed diagonal linear differential equation which can be obtained for integrally separated systems by a change of variables from a perturbed triangular differential equation but with less control on the size of the perturbation. This was overcome in [11] where perturbed triangular differential equations were considered directly. The perturbed triangular differential equation was shown to exist and first order bounds on the perturbation of the coefficient matrix function were obtained in [8] starting from the backward error analysis for the perturbed triangular factors as in (2.3). However, obtaining sharp bounds on the perturbation of the triangular coefficient matrix function is difficult. The present analysis removes the step of obtaining the perturbed triangular *differential equation* and bounding its perturbation. In addition, the analysis in [9] and [11] was based upon the nonlinear variation of constants formula and the contraction mapping principle. The splitting of the differential equation that brings the perturbed triangular differential equation to triangular employed in both [9] and [11] corresponds to the perturbed Jacobian (essentially by approximating a matrix by its diagonal elements) that we use in our analysis here. However, an improved perturbed Jacobian in which only "small" quantities are ignored is straightforward to implement numerically.

We next establish the bounds (4.2), (4.3), and (4.5).

4.1. Linearization and approximate Jacobian. We have from (3.2) that the derivative of G_1 with respect to Q_n in the direction $\{V_k\}_{k=1}^\infty$ is given by

$$D_{Q_n}(G_1(\{Q_k\}_{k=1}^\infty)(\{V_k\}_{k=1}^\infty))_n = \texttt{slow}(Q_{n+1}^T[R_n + E_n]V_n),$$

and the derivative of G_1 with respect to Q_{n+1} in the direction $\{V_k\}_{k=1}^\infty$ is

$$D_{Q_{n+1}}(G_1(\{Q_k\}_{k=1}^\infty)(\{V_k\}_{k=1}^\infty))_n = \texttt{slow}(V_{n+1}^T[R_n + E_n]Q_n),$$

while the directional derivative of G_2 with respect to Q_{n+1} is

$$D_{Q_{n+1}}(G_2(\{Q_k\}_{k=1}^\infty)(\{V_k\}_{k=1}^\infty))_n = \texttt{upp}(V_{n+1}Q_{n+1}^T + Q_{n+1}V_{n+1}^T).$$

Then we have, since $x_0 = \{I\}_{k=1}^\infty$,

$$(G_1'(x_0)(\{V_k\}_{k=1}^\infty))_n = \texttt{slow}(V_{n+1}^T[R_n + E_n]) + \texttt{slow}([R_n + E_n]V_n)$$

and

$$(G_2'(x_0)(\{V_k\}_{k=1}^{\infty}))_n = \texttt{upp}(V_{n+1} + V_{n+1}^T).$$

We will employ an approximate Jacobian Γ by using a subset of the terms from the exact Jacobian relative to the variation in G_1, but will use the exact Jacobian relative to the variation in G_2. In particular, we take Γ_1 as

$$(\Gamma_1(\{V_k\}_{k=1}^{\infty}))_n = \texttt{slow}(V_{n+1}^T \operatorname{diag}(R_n)) + \texttt{slow}(\operatorname{diag}(R_n)V_n) \text{ and } \Gamma_2 = G_2'(x_0). \tag{4.9}$$

Note that for $i > j$, the (i,j) element of

$$D_{Q_n}(G_1(\{Q_k^{(0)}\}_{k=1}^{\infty})(\{V_k\}_{k=1}^{\infty}))_n + D_{Q_{n+1}}(G_1(\{Q_k^{(0)}\}_{k=1}^{\infty})(\{V_k\}_{k=1}^{\infty}))_n$$

is

$$\sum_{k=1}^{j}(V_{n+1})_{ki}(R_n)_{kj} + \sum_{k=1}^{m}(V_{n+1})_{ki}(E_n)_{kj} + \sum_{k=i}^{m}(R_n)_{ik}(V_n)_{kj} + \sum_{k=1}^{m}(E_n)_{ik}(V_n)_{kj} \tag{4.10}$$

for $n = 0, 1, \ldots,$ with the understanding that $V_0 = 0$. For the approximate Jacobian Γ, we replace (4.10) with

$$(V_{n+1})_{ji}(R_n)_{jj} + (R_n)_{ii}(V_n)_{ij}. \tag{4.11}$$

This then results in a system in which the V_n terms may be considered as known and we must solve for the terms V_{n+1}. To this end, consider the system of equations of the form

$$(V_{n+1})_{ji}(R_n)_{jj} = -(R_n)_{ii}(V_n)_{ij} + (W_n)_{ij} \tag{4.12}$$

for $i > j$ and $n = 0, 1, \ldots,$ with $V_0 = 0$.

We note here that for the bounds in (3.3) and (3.4) we have $(G_2(x_0))_n = 0$ since $x_0 = \{I\}_{k=1}^{\infty}$ which implies

$$D_{Q_{n+1}}(G_1(\{Q_k^{(0)}\}_{k=1}^{\infty})(\{V_k\}_{k=1}^{\infty}))_n := \texttt{upp}(V_{n+1} + V_{n+1}^T) = 0$$

so that V_{n+1} is a real skew-symmetric matrix for all n. This simplifies bounding (3.3) and (3.4) since in this case we can replace the term $(V_n)_{ij}$ in (4.12) with $-(V_n)_{ji}$ so that the system becomes diagonal.

4.2. Bounds on $\|\Gamma^{-1}G(x_0)\|$. We first prove the following lemma to obtain the bound η on $\|\Gamma^{-1}G(x_0)\|$ given in (4.2). We first note for $x_0 = \{I\}_{k=1}^{\infty}$ and G given in (3.1) and (3.2), $(G_1(x_0))_n = \texttt{slow}(E_n)$ and $(G_2(x_0))_n = \texttt{upp}(0)$.

LEMMA 4.2. *For the norm $\|\cdot\|$ defined for sequences of matrices by $\|\{V_k\}_{k=1}^{\infty}\| = \sup_k \|V_k\|_F$, we have $\|\Gamma^{-1}G(x_0)\| \le \eta$ for G defined in* (3.1) *and* (3.2), *Γ defined in* (4.9), (4.10), *and* (4.11), *$x_0 = \{I\}_{k=1}^{\infty}$, and η given in* (4.2).

Proof. To determine this bound, we consider the linear system $\Gamma V = G(x_0)$, where $V := \{V_k\}_{k=1}^{\infty}$ with the understanding that $V_0 = 0$ and $Q_0 = I$, and next derive bounds on the V_n. We will take advantage of the fact that $G_2(x_0) = 0$. We have for $i > j$ that $(W_n)_{ij} = (E_n)_{ij}$ in (4.12) so that

$$(V_{n+1})_{ji} = \frac{(R_n)_{ii}(V_n)_{ji} + (E_n)_{ij}}{(R_n)_{jj}}. \tag{4.13}$$

By the discrete variation of parameters formula, we have

$$(V_{n+1})_{ji} = \sum_{k=1}^{n} (\Psi_{nk})_{ij} \frac{(E_{k-1})_{ij}}{(R_{k-1})_{jj}} + \frac{(E_n)_{ij}}{(R_n)_{jj}}, \quad (\Psi_{nk})_{ij} = \frac{(R_n)_{ii}}{(R_n)_{jj}} \cdots \frac{(R_k)_{ii}}{(R_k)_{jj}} \tag{4.14}$$

so that by (3.6)

$$\begin{aligned} |(V_{n+1})_{ji}| &\le \left[\frac{1}{\Omega_{ij}}(1+\lambda_{ij}^{-1}+\cdots\lambda_{ij}^{-n})+1\right]\cdot\frac{|E_{ij}|}{R_{jj}} \\ &\le \left[\frac{\lambda_{ij}}{\Omega_{ij}(\lambda_{ij}-1)}+1\right]\cdot\frac{|E_{ij}|}{R_{jj}} = \Lambda_{ij}\frac{|E_{ij}|}{R_{jj}}, \end{aligned} \tag{4.15}$$

where $|E_{ij}|/R_{jj} = \sup_n |(E_n)_{ij}|/(R_n)_{jj}$. Then to bound η in (3.3), we have

$$\begin{aligned} \eta &\le \sup_n \|V_{n+1}\|_F = \sup_n \sqrt{2}\left(\sum_{j=1}^{m-1}\sum_{i=j+1}^{m}(V_{n+1})_{ji}^2\right)^{1/2} \\ &\le \sqrt{2}\left(\sum_{j=1}^{m-1}\sum_{i=j+1}^{m}\left(\Lambda_{ij}\frac{|E_{ij}|}{R_{jj}}\right)^2\right)^{1/2}. \qquad \square \end{aligned} \tag{4.16}$$

4.3. Bounds on $\|\Gamma^{-1}G'(x_0) - I\|$. We next prove the following lemma to obtain the bound δ on $\|\Gamma^{-1}G'(x_0) - I\|$ given in (4.3).

LEMMA 4.3. *Under the same assumptions as in Lemma* 4.2, $\|\Gamma^{-1}G'(x_0)-I\| \le \delta$ *for δ given in* (4.3).

Proof. If we rewrite $\Gamma^{-1}G'(x_0) - I = \Gamma^{-1}(G'(x_0) - \Gamma)$, then for $i > j$ we have,

$$\begin{aligned} (W_n)_{ij} = &\sum_{k=1}^{m}(X_{n+1})_{ki}(E_n)_{kj} + \sum_{k=1}^{m}(E_n)_{ik}(X_n)_{kj} + \sum_{k=1}^{j-1}(X_{n+1})_{ki}(R_n)_{kj} \\ &+ \sum_{k=i+1}^{m}(R_n)_{ik}(X_n)_{kj}. \end{aligned} \tag{4.17}$$

Then

$$(V_{n+1})_{ji} = \frac{(R_n)_{ii}(V_n)_{ji} + (W_n)_{ij}}{(R_n)_{jj}}. \tag{4.18}$$

Proceeding as in (4.14) and (4.15), we have

$$|(V_{n+1})_{ji}| \le \left[\frac{\lambda_{ij}}{\Omega_{ij}(\lambda_{ij}-1)}+1\right]\cdot\frac{|W_{ij}|}{R_{jj}} = \Lambda_{ij}\frac{|W_{ij}|}{R_{jj}}, \tag{4.19}$$

where $|W_{ij}|/R_{jj} = \sup_n |(W_n)_{ij}|/(R_n)_{jj}$.

To compute the norm, we take the supremum over all sequences of matrices $\{X_k\}$ such that $\sup_k \|X_k\|_F = 1$. Then by the Cauchy–Schwartz inequality using (4.17),

$$\frac{|W_{ij}|}{R_{jj}} \le \sup_n (R_n)_{jj}^{-1}\left[\|(E_n)_{\cdot j}\|_2 + \|(E_n)_{i\cdot}\|_2 + \left(\sum_{k=1}^{j-1}(R_n)_{kj}^2\right)^{1/2} + \left(\sum_{k=i+1}^{m}(R_n)_{ik}^2\right)^{1/2}\right], \tag{4.20}$$

where $(E_n)_{\cdot j}$ is the jth column of E_n and $(E_n)_{i\cdot}$ is the ith row of E_n. Then

$$\delta \le \sup_n \|V_{n+1}\|_F = \sup_n \sqrt{2}\left(\sum_{j=1}^{m-1}\sum_{i=j+1}^{m}(V_{n+1})_{ji}^2\right)^{1/2} \le \sqrt{2}\left(\sum_{j=1}^{m-1}\sum_{i=j+1}^{m}\left(\Lambda_{ij}\frac{|W_{ij}|}{R_{jj}}\right)^2\right)^{1/2}. \qquad \square \tag{4.21}$$

4.4. Bounds on $\|\Gamma^{-1}G''(x)\|$. Before proceeding with the second derivative bounds, we observe that $G(\{Q_k\}_{k=1}^{\infty})$ is quadratic, so G'' is constant. The bounds here are somewhat different than the previous bounds since $G_2''(x) \neq 0$, so we do not have that the V_n are skew-symmetric.

LEMMA 4.4. *Under the same assumptions as in Lemma* 4.2, $\|\Gamma^{-1}G''(x)\| \le K$ *for any x where K given in* (4.5).

Proof. Here we have for $i > j$,

$$(W_n)_{ij} = [X_{n+1}^T(R_n + E_n)Y_n + Y_{n+1}^T(R_n + E_n)X_n]_{ij} \tag{4.22}$$

in (4.12) which gives

$$(V_{n+1})_{ji} = \frac{-(R_n)_{ii}(V_n)_{ij} + (W_n)_{ij}}{(R_n)_{jj}}. \tag{4.23}$$

For $i \le j$, we have for all n that

$$(V_{n+1})_{ij} + (V_{n+1})_{ji} = [X_{n+1}Y_{n+1}^T + Y_{n+1}X_{n+1}^T]_{ij}. \tag{4.24}$$

Then combining (4.23) and (4.24), we have for $i > j$,

$$\begin{aligned}(V_{n+1})_{ji} &= \frac{(R_n)_{ii}[(V_n)_{ji} - [X_nY_n^T + Y_nX_n^T]_{ji}] + (W_n)_{ij}}{(R_n)_{jj}} \\ &=: \frac{(R_n)_{ii}(V_n)_{ji}}{(R_n)_{jj}} + (\tilde{W}_n)_{ij}\end{aligned} \tag{4.25}$$

and

$$\begin{aligned}(V_{n+1})_{ij} &= \frac{(R_n)_{ii}(V_n)_{ij} - (W_n)_{ij}}{(R_n)_{jj}} + [X_{n+1}Y_{n+1}^T + Y_{n+1}X_{n+1}^T]_{ji} \\ &=: \frac{(R_n)_{ii}(V_n)_{ij}}{(R_n)_{jj}} + (\overline{W}_n)_{ij}.\end{aligned} \tag{4.26}$$

Thus, for $i > j$,

$$|(V_{n+1})_{ji}| \le \Lambda_{ij} \cdot |\tilde{W}_{ij}| \text{ and } |(V_{n+1})_{ij}| \le \Lambda_{ij} \cdot |\overline{W}_{ij}|. \tag{4.27}$$

If X_n, Y_n, X_{n+1}, and Y_{n+1} are all matrices with Frobenius norm equal to one, then a simple application of the Cauchy–Schwarz inequality applied to (4.24) with $i = j$ implies $\sum_{i=1}^m (V_{n+1})_{ii}^2 \le 1$, and similarly, we bound $|\tilde{W}_{ij}|$ and $|\overline{W}_{ij}|$ as

$$\begin{aligned}|\tilde{W}_{ij}| &\le \sup_n \frac{1}{(R_n)_{jj}} + 2(\|R_n^{(jj)}\|_F + \|E_n^{(jj)}\|_F) \text{ and} \\ |\overline{W}_{ij}| &\le \sup_n 2(\|R_n^{(jj)}\|_F + \|E_n^{(jj)}\|_F) + 1,\end{aligned} \tag{4.28}$$

where $R_n^{(jj)} = (R_n)_{jj}^{-1} R_n$ and $E_n^{(jj)} = (R_n)_{jj}^{-1} E_n$. Thus, K in (3.5) is bounded as

$$K \le \left(1 + \sum_{j=1}^{m-1} \sum_{i=j+1}^{m} \Lambda_{ij}^2 (|\tilde{W}_{ij}|^2 + |\overline{W}_{ij}|^2) \right)^{1/2} . \qquad \square \tag{4.29}$$

5. Componentwise bounds. To obtain componentwise bounds, we make a change of variables and use a different, weighted norm. First, rewrite (3.1) and (3.2) in terms of the new unknown $Z_n = Q_n - I$ so we have

$$\begin{aligned} (G_1(\{Z_k\}_{k=1}^\infty))_n &= \mathtt{slow}((Z_{n+1}^T + I)[R_n + E_n](Z_n + I)) \\ (G_2(\{Z_k\}_{k=1}^\infty))_n &= \mathtt{upp}((Z_{n+1} + I)(Z_{n+1}^T + I) - I) \end{aligned} \tag{5.1}$$

and employ the initial guess for the perturbed Newton iteration of $Z_n^{(0)} = 0$ for all n. Then replace the norm $\sup_n \|Q_n - I\|_F$ with the norm

$$\|Z\| \equiv \|\{Z_n\}_{n=1}^\infty\| = \sup_n \sup_{i,j} |\omega_{ij} (Z_n)_{ij}|, \;\; \omega_{ij} > 0, \tag{5.2}$$

where we will determine the weights ω_{ij} so that at least approximately $|\omega_{ij}(Z_n)_{ij}| = |\omega_{kl}(Z_{n'})_{kl}|$ independent of i, j, k, l, and n, n'. Then $\|Z\| \le r_0$ implies that $|(Z_n)_{ij}| \le \omega_{ij}^{-1} r_0 =: \rho_{ij}$, and then for $i \le j$,

(5.3)

$$\begin{aligned} |(\overline{R}_n - R_n)_{ij}| \le |(E_n)_{ij}| &+ \sum_{k=i}^{m} |(R_n)_{ik}| \rho_{kj} + \sum_{k=1}^{j} \rho_{ki} |(R_n)_{kj}| + \sum_{k=1}^{m-1} \sum_{l=k}^{m} \rho_{ki} |(R_n)_{kl}| \rho_{lj} \\ &+ \sum_{k=1}^{m} |(E_n)_{ik}| \rho_{kj} + \sum_{k=1}^{m} \rho_{ki} |(E_n)_{kj}| + \sum_{k=1}^{m} \sum_{l=1}^{m} \rho_{ki} |(E_n)_{kl}| \rho_{lj}. \end{aligned}$$

We note that these bounds are useful in obtaining bounds on Lyapunov exponents and the endpoints of Sacker–Sell spectral intervals (see [9]).

We consider here a simple way of choosing the weights ω_{ij}. Consider the bound (4.15), where for $i > j$, $|(V_{n+1})_{ji}| \le \Lambda_{ij} \frac{|E_{ij}|}{R_{jj}} =: \beta_{ij}$. Then for some $k > l$, $\beta_{kl} = \max_{i>j} \beta_{ij}$, so if we let

$$\omega_{ij} = \beta_{kl} / \beta_{ij}, \tag{5.4}$$

then $\omega_{ij} \ge 1$ and $|\omega_{ij}(V_{n+1})_{ji}| \le \beta_{kl}$ for all $i > j$, and we define $\omega_{ij} = \omega_{ji}$ for $i < j$. To define ω_{ii} for $i = 1, \ldots, m$, note that by orthogonality, $(Z_n)_{ii}((Z_n)_{ii} + 2) = \sum_{i \ne j} (Z_n)_{ij}^2 =: C_i$ so that by the quadratic formula, $(Z_n)_{ii} = \sqrt{1 + C_i} - 1$. Ultimately, we will bound $|Z_{ij}| \le \omega_{ij}^{-1} r_0$, so using the approximation $\sqrt{1+x} - 1 \approx \frac{x}{2}$ we set

$$\omega_{ii} = 2 \Big[\sum_{i \ne j} \omega_{ij}^{-2} \Big]^{-1}, \;\; i = 1, \ldots, m.$$

More sophisticated choices for the ω_{ij} are possible as are weights that depend on n.

Lemma 5.1. *For the norm given in* (5.2) *with the weights defined in* (5.13)*, G defined in* (3.1) *and* (3.2)*, Γ defined in* (4.9), (4.10)*, and* (4.11)*, and initial guess $x_0 = \{I\}_{k=1}^\infty$, we obtain the following bounds:*

(i) $\|\Gamma^{-1}G(x_0)\| \le \eta := \max_{i>j} \omega_{ij}\Lambda_{ij}\frac{|E_{ij}|}{R_{jj}}$,

(ii) $\|\Gamma^{-1}G'(x_0) - I\| \le \delta := \max_{i>j} \omega_{ij}\Lambda_{ij}\frac{|W_{ij}|}{R_{jj}}$,

(iii) $\|\Gamma^{-1}G''(x)\| \le K := \max\{K_1, K_2, K_3\}$,

where

$$K_1 = \max_{1\le i\le m} \omega_{ii}K_{ii},\ \ K_2 = \max_{i>j} \omega_{ij}\Lambda_{ij}K_{ji},\ \ K_3 = \max_{i>j} \omega_{ij}\Lambda_{ij}K_{ij} \tag{5.5}$$

and K_{ii}, K_{ji}, and K_{ij} are defined in (5.9), (5.10), and (5.11), respectively.

Proof. The bound for η is straightforward since each V_n is skew-symmetric,

$$\eta = \max_{i>j} \omega_{ij}\Lambda_{ij}\frac{|E_{ij}|}{R_{jj}}. \tag{5.6}$$

To compute the bound on δ, we take the supremum over all sequences of matrices $\{X_k\}$ such that $\omega_{ij}|(X_k)_{ij}| = 1$ for all (i, j). Then by the Cauchy–Schwartz inequality using (4.17),

$$\frac{|W_{ij}|}{R_{jj}} \le \sup_n\ (R_n)^{-1}_{jj} \left[\|\Omega^{-1}_{\cdot i}\|_2 \cdot \|(E_n)_{\cdot j}\|_2 + \|(E_n)_{i\cdot}\|_2 \cdot \|\Omega^{-1}_{\cdot j}\|_2 + \sum_{k=1}^{j-1} |\omega^{-1}_{ki}(R_n)_{kj}| + \sum_{k=i+1}^{m} |(R_n)_{ik}\omega^{-1}_{kj}|\right], \tag{5.7}$$

where $(E_n)_{\cdot j}$ is the jth column of E_n, $(E_n)_{i\cdot}$ is the ith row of E_n, and $\Omega^{-1}_{\cdot j}$ is the jth column of the matrix Ω^{-1} whose (i, j) element is ω^{-1}_{ij}. Thus,

$$\delta = \max_{i>j} \omega_{ij}\Lambda_{ij}\frac{|W_{ij}|}{R_{jj}} \tag{5.8}$$

using the bound for $|W_{ij}|/R_{jj} = \sup_n |(W_n)_{ij}|/(R_n)_{jj}$ in (5.7).

We obtain the bound for K using (4.22), (4.25), (4.26), and (4.27). First, from (4.24) we have for $i = j$, $2(V_{n+1})_{ii} = [X_{n+1}Y^T_{n+1} + Y_{n+1}X^T_{n+1}]_{ii}$ so that for $|\omega_{ij}(X_{n+1})_{ij}| = 1$ and $|\omega_{ij}(Y_{n+1})_{ij}| = 1$ for all (i, j) we have

$$|(V_{n+1})_{ii}| \le \sum_{k=1}^{m} \omega^{-2}_{ik} =: K_{ii}. \tag{5.9}$$

Then to obtain the bounds analogous to (4.27), we have for $i > j$,

$$|\tilde{W}_{ij}| \le \sup\nolimits_n \frac{2}{(R_n)_{jj}} \sum_{k=1}^{m} \omega^{-1}_{ik}\omega^{-1}_{jk} + 2\sum_{k=1}^{m}\sum_{l=1}^{m} \omega^{-1}_{ki}\left[|(R^{(jj)}_n)_{kl}| + |(E^{(jj)}_n)_{kl}|\right]\omega^{-1}_{lj} =: K_{ji} \tag{5.10}$$

and

$$|\overline{W}_{ij}| \le \sup\nolimits_n 2\sum_{k=1}^{m} \omega^{-1}_{ik}\omega^{-1}_{jk} + 2\sum_{k=1}^{m}\sum_{l=1}^{m} \omega^{-1}_{ki}\left[|(R^{(jj)}_n)_{kl}| + |(E^{(jj)}_n)_{kl}|\right]\omega^{-1}_{lj} =: K_{ij} \tag{5.11}$$

from which the bound for K follows. ☐

Summarizing, we have the following theorem that gives componentwise bounds.

THEOREM 5.2. *If for the bounds on η, δ, and K in Lemma* 5.1 *we have $\delta < 1$ and $h := \frac{\eta K}{(1-\delta)^2} < \frac{1}{2}$, then for $r_0 = \frac{2\eta}{(1-\delta)(1+\sqrt{1-2h})}$,*

$$\sup_n |(Z_n)_{ij}| \equiv \sup_n |(Q_n - I)_{ij}| \leq \omega_{ij}^{-1} r_0 \equiv \rho_{ij}, \tag{5.12}$$

where for $i > j$,

$$\omega_{ij}^{-1} = \frac{\Lambda_{ij} \frac{|E_{ij}|}{R_{jj}}}{\max_{k<l} \Lambda_{kl} \frac{|E_{kl}|}{R_{ll}}}, \;\; \omega_{ji}^{-1} = \omega_{ij}^{-1}, \tag{5.13}$$

$\omega_{ii}^{-1} = 1$, $i = 1, \dots, m$, Λ_{ij} is defined in (3.7), *and $\frac{|E_{ij}|}{R_{jj}} = \sup_n |(E_n)_{ij}|/(R_n)_{jj}$. Moreover, the bound* (5.3) *on the error in the components of the upper triangular factor holds.*

6. Numerical results. We next outline how these ideas may be implemented to perform an a posterior error analysis. We then apply these ideas to a model problem that allows us to modify the strength of the integral separation and the nonnormality in the triangular factor and to a problem modeled after one in stability analysis.

6.1. A posteriori error analysis. We will obtain componentwise bounds using the weights and norm developed in section 5. In addition, we will compare the perturbed Jacobian we have used in the analysis, which is essentially a diagonal approximation of the Jacobian, with a perturbed Jacobian, in which only "small" terms are neglected. Recall from (3.2) that

$$(G_1(\{Q_k\}_{k=1}^\infty))_n = \texttt{slow}(Q_{n+1}^T [R_n + E_n] Q_n),$$

which has first derivative $(G_1'(\{I\}_{k=1}^\infty)\{V_k\}_{k=1}^\infty)_n = \texttt{slow}(V_{n+1}^T[R_n+E_n]+[R_n+E_n]V_n)$ which we approximated with the "diagonal approximation,"

$$(\Gamma_1\{V_k\}_{k=1}^\infty)_n := \texttt{slow}(V_{n+1}^T \operatorname{diag}(R_n) + \operatorname{diag}(R_n) V_n).$$

In particular, we will also consider the alternate "triangular approximation,"

$$(\tilde{\Gamma}_1\{V_k\}_{k=1}^\infty)_n := \texttt{slow}(V_{n+1}^T R_n + R_n V_n).$$

For the calculation of the bound on the first Newton step, η, for both "approximations" when $x_0 = \{I\}_{k=1}^\infty$, $G_1(x_0)_n = \texttt{slow}(E_n)$ and $G_2(x_0)_n = 0$ and the iteration is

$$\texttt{slow}(V_{n+1} D_n) = [\texttt{slow}(D_n V_n) + \texttt{slow}(E_n)], \;\; n = 0, 1, \dots, \;\; V_0 = 0,$$

where $D_n := \operatorname{diag}(R_n)$ for the "diagonal approximation" and $D_n := R_n$ for the "triangular approximation" since $\texttt{upp}(V_{n+1} + V_{n+1}^T) = 0$ implies $V_{n+1} = -V_{n+1}^T$.

For the calculation of the bound δ that measures the difference between the exact and the perturbed Jacobian, we have

$$\begin{aligned} &[(G_1'(x_0) - \Gamma_1))\{X_k\}_{k=1}^\infty]_n \\ &\quad = \texttt{slow}(X_{n+1}^T [R_n - \operatorname{diag}(R_n) + E_n] + [R_n - \operatorname{diag}(R_n) + E_n] X_n) \end{aligned} \tag{6.1}$$

and

$$[(G_1'(x_0) - \tilde{\Gamma}_1))\{X_k\}_{k=1}^\infty]_n = \texttt{slow}(X_{n+1}^T E_n + E_n X_n), \tag{6.2}$$

and the iteration is similar to that for η since the V_n are still skew-symmetric.

For the calculation of the second derivative bound K, the V_n are no longer skew-symmetric, and we have the iteration

$$\left\{\begin{array}{rcl} \mathtt{slow}(V_{n+1}^T D_n) & = & [-\mathtt{slow}(D_n V_n) + \mathtt{slow}(X_{n+1}^T (R_n + E_n) Y_n \\ & & +Y_{n+1}^T (R_n + E_n) X_n)], \\ \mathtt{upp}(V_{n+1} + V_{n+1}^T) & = & \mathtt{upp}(X_{n+1} Y_{n+1}^T + Y_{n+1} X_{n+1}^T). \end{array}\right. \tag{6.3}$$

To obtain bounds using the weighted norm in (5.2), first consider the iteration to obtain η. We actually form

$$\mathtt{slow}(V_{n+1}) = \mathtt{slow}(\{|D_n| \cdot V_n + |E_n|\} \cdot |D_n^{-1}|), \quad n = 0, 1, \dots,$$

where the notation $|X|$ of a matrix X is used to the denote the matrix $|X|$ such that $|X|_{ij} = |X_{ij}|$. We then calculate $\eta := \|V\|$ for $V = \{V_n\}_{n=0}$ using the weighted norm (5.2). To determine δ, we replace $\mathtt{slow}(|E_n|)$ with the analogous quantity using either (6.1) or (6.2), depending upon which perturbed Jacobian is being employed. In addition, we take $X = \{X_n\}_{n=0}$ with $\|X\| = 1$, in particular $(X_n)_{ij} = \omega_{ij}^{-1}$. When finding the bound K, we solve the iteration

$$\left\{\begin{array}{l} \mathtt{slow}(V_{n+1}^T) = \mathtt{slow}(\{|D_n| \cdot V_n + X_{n+1}^T (|R_n| + |E_n|) Y_n + Y_{n+1}^T (|R_n| + |E_n|) X_n\} \\ \qquad\qquad\qquad \cdot |D_n^{-1}|), \\ \mathtt{supp}(V_{n+1}^T) = \mathtt{slow}(V_{n+1}^T)^T + \mathtt{supp}(X_{n+1} Y_{n+1}^T + Y_{n+1} X_{n+1}^T), \\ \mathrm{diag}(V_{n+1}) = \dfrac{1}{2} \mathrm{diag}(X_{n+1} Y_{n+1}^T + Y_{n+1} X_{n+1}^T), \end{array}\right. \tag{6.4}$$

where $(X_n)_{ij} = \omega_{ij}^{-1}$, $(Y_n)_{ij} = \omega_{ij}^{-1}$, and $\mathtt{supp}$ denotes the strictly upper triangular part of a matrix.

6.2. Example 1. We now consider an example that illustrates the dependence on the degree of nonnormality and on the strength of integral separation and shows the sharpness of the results we have obtained. We focus on the product of perturbed triangular systems with $m = 3$ so that in general R_n is given by

$$R_n = \begin{pmatrix} (R_n)_{11} & (R_n)_{12} & (R_n)_{13} \\ 0 & (R_n)_{22} & (R_n)_{23} \\ 0 & 0 & (R_n)_{33} \end{pmatrix}, \tag{6.5}$$

where we consider $(R_n)_{11} = 4 + \kappa \sin(\zeta n)$, $(R_n)_{22} = 3 - \sin(\sqrt{2}\zeta n)$, $(R_n)_{33} = 2 + \kappa \sin(2\zeta n)$, and $\gamma = R_{12} = R_{23} = R_{13}$ independent of n. We change κ and ζ to vary the strength of integral separation, and we vary γ to change the off-diagonal entries and vary the strength of nonnormality. We generate random E_n such that $|(E_n)_{ij}| \le \epsilon$ using the MATLAB command `2*rand-1`. To determine the quality of the bounds we obtain, we compare them with $|(Q_n - I)_{ij}|$, where Q_n is such that $Q_{n+1}\overline{R}_n = [R_n + E_n]Q_n$ for $n = 0, 1, \dots, N$, with $Q_0 = I$. As a measure of the quality of our bounds, we denote by $\mathtt{Diag} = \sup_{i \ne j} \frac{\rho_{ij}}{\sup_n |(Q_n)_{ij}|}$ and $\mathtt{Off} = \sup_i \frac{\rho_{ii}}{\sup_n |(Q_n)_{ii} - 1|}$, where ρ_{ij} is the bound (5.12) in Theorem 5.2 so that $\mathtt{Diag} \ge 1$ and $\mathtt{Off} \ge 1$, with a value of 1 meaning that the bound is sharp. We consider both the diagonal approximation of the Jacobian which we denote by `diag` and the triangular approximation of the Jacobian which we denote by `tri`.

In Table 6.1 we illustrate the results of some of our numerical experiments; in each row we report on the average value obtained over 10 sequences of matrices,

Table 6.1
Error in the approximate Q varying the degree of nonnormality and integral separation, method, and tolerance.

$N = 10^5$

ζ	κ	γ	ϵ	Meth	η	K	δ	r_0	Diag	Off
1	1	1	$1E-4$	tri	$2E-4$	$3.0E1$	$6E-4$	$2E-4$	$2.3E0$	$2.4E0$
1	1	10	$1E-4$	tri	$8E-4$	$2.1E2$	$2E-3$	$8E-4$	$2.8E0$	$8.7E0$
0.2	0.5	1	$1E-4$	tri	$7E-4$	$1.1E2$	$2E-3$	$7E-4$	$2.7E0$	$2.1E0$
1	1	1	$1E-6$	tri	$2E-6$	$3.0E1$	$6E-6$	$2E-6$	$2.2E0$	$2.4E0$
1	1	10	$1E-6$	tri	$7E-6$	$2.1E2$	$2E-5$	$7E-6$	$2.4E0$	$7.9E0$
0.2	0.5	1	$1E-6$	tri	$7E-6$	$1.1E2$	$2E-5$	$7E-6$	$2.6E0$	$2.0E0$
0.2	0.5	10	$1E-6$	tri	$3E-5$	$6.7E2$	$7E-5$	$3E-5$	$2.3E0$	$8.4E0$
0.1	0.5	10	$1E-6$	tri	$9E-5$	$1.3E3$	$2E-4$	$9E-5$	$4.1E0$	$9.1E0$
0.2	0.5	10	$1E-8$	tri	$3E-7$	$6.7E2$	$7E-7$	$3E-7$	$2.3E0$	$8.1E0$
0.1	0.5	10	$1E-8$	tri	$8E-7$	$1.3E3$	$2E-6$	$8E-7$	$3.5E0$	$8.5E0$
0.1	1	10	$1E-8$	tri	$5E-6$	$2.5E3$	$7E-6$	$5E-6$	$7.1E0$	$1.2E1$
1	1	1	$1E-4$	diag	$2E-4$	$2.5E1$	$9E-1$	$--$	$--$	$--$
1	1	10	$1E-4$	diag	$2E-4$	$7.9E1$	$9E0$	$--$	$--$	$--$
0.2	0.5	1	$1E-4$	diag	$5E-4$	$8.5E1$	$1.2E0$	$--$	$--$	$--$
1	1	1	$1E-6$	diag	$2E-6$	$2.5E1$	$9E-1$	$2E-5$	$2.4E2$	$2.5E1$
1	1	10	$1E-6$	diag	$2E-6$	$7.9E1$	$9E0$	$--$	$--$	$--$
0.2	0.5	1	$1E-6$	diag	$5E-6$	$8.5E1$	$1.2E0$	$--$	$--$	$--$
1	1	1	$1E-8$	diag	$2E-8$	$2.5E1$	$9E-1$	$2E-7$	$1.2E2$	$2.4E1$
1	1	10	$1E-8$	diag	$2E-8$	$7.9E1$	$9E0$	$--$	$--$	$--$
0.2	0.5	1	$1E-8$	diag	$5E-8$	$8.5E1$	$1.2E0$	$--$	$--$	$--$

R_n with randomly generated error matrices, E_n, for $n = 0, \ldots, N$. We only report on parameter values for which all 10 trials could successfully provide an error bound. In this case we list the average values of the bound K on $\|\Gamma^{-1}G''(x_0)\|$, the bound δ on $\|\Gamma^{-1}G'(x_0) - I\|$, and the radius of the Newton ball $r_0 = 2\eta/((1-\delta)(1+\sqrt{1-2h}))$, provided $h = \eta K/(1-\delta)^2 < 1/2$ for all 10 trials. Decreasing ζ and increasing κ tends to decrease the strength of the integral separation, while increasing γ clearly increases in the nonnormality in the triangular factor. For the "triangular approximation" of the Jacobian, results are obtained as the problems become more difficult as long as the size of the perturbation is small enough. In addition, the bounds obtained are within an order of magnitude for the parameter values reported in Table 6.1. Sharper bounds might be obtained by an improved choice of the weights, ω_{ij}. For the "diagonal approximation" of the Jacobian, we were not able to obtain bounds for the more difficult problems except for smaller ϵ and γ, and the bounds obtained were not as sharp.

6.3. Example 2. For our next example, we consider a prototype model of mistuning in N rotating blades of the form

$$\ddot{u}_j(t) + q_j(t)u_j(t) = \epsilon(u_{j+1} - 2u_j + u_{j-1}) + \epsilon(\dot{u}_{j+1} - 2\dot{u}_j + \dot{u}_{j-1}), \;\; j = 1, \ldots, N,$$

with periodic boundary conditions so that $u_0 \equiv u_N$ and $u_1 \equiv u_{N+1}$. The left-hand side of the equation contains the structural inertia and stiffness terms, while the right-hand side contains the forces due to aerodynamic coupling under the assumption of nearest neighbor coupling and that the unsteadiness is of low frequency. This is similar to a model employed in [4]; see also [3]. For our purposes here, we consider the $q_j(t)$ of the Mathieu type, in particular, $q_j(t) = \pi^2 + \gamma_j \cos(2\pi t)$, and take $N = 3$ with $\gamma_1 = 30$, $\gamma_2 = 20$, and $\gamma_3 = 10$. We employ a variable step differential equation

TABLE 6.2
Error estimates in the approximation of Q for different local error tolerances and time intervals.

T	TOL	N	$r_0 \equiv \sup_{i\neq j} \rho_{ij}$	$\inf_{i\neq j} \rho_{ij}$	$\sup_i \rho_{ii}$	$\inf_i \rho_{ii}$
1	$1E-4$	34	$4E-3$	$1E-4$	$3E-7$	$8E-8$
1	$1E-5$	66	$3E-4$	$1E-5$	$2E-9$	$5E-10$
1	$1E-6$	97	$3E-5$	$1E-6$	$2E-11$	$6E-12$
1	$1E-7$	155	$3E-6$	$1E-7$	$2E-13$	$5E-14$
10	$1E-6$	988	$6E-4$	$1E-6$	$5E-11$	$8E-13$
10	$1E-7$	1532	$6E-5$	$1E-7$	$5E-13$	$1E-14$
100	$1E-6$	9898	$6E-4$	$1E-6$	$5E-11$	$8E-13$
100	$1E-7$	15302	$6E-5$	$1E-7$	$5E-13$	$1E-14$

solver based upon `rkf45` to approximate the local fundamental matrix solutions, the $A_n + F_n$, and use the local error tolerance TOL to estimate $\|F_n\|$. In our calculations we consider $\epsilon = 10^{-1}$ and report on the error in the orthogonal factor as a function of different local error tolerances. After rewriting the differential equation as a first order system of the form $\dot{x} = \tilde{A}(t)x$, we form the $A_n + F_n$ as the solution of the differential equation

$$\dot{X}(t; t_n) = \tilde{A}(t)X(t; t_n), \;\; t > t_n, \;\; X(t_n; t_n) = I$$

at time $t = t_{n+1}$ so that $A_n + F_n := X(t_{n+1}; t_n)$. We then form $\overline{Q}_{n+1}R_n = [A_n + F_n]\overline{Q}_n$ using the modified Gram–Schmidt procedure. We bound the elements of $E_n = -\overline{Q}_{n+1}^T F_n \overline{Q}_n$ using

$$|(E_n)_{ij}| \leq \mathtt{TOL} \cdot (|\overline{Q}_{n+1}|^T \cdot \mathbf{1} \cdot |\overline{Q}_n|)_{ij},$$

where $|\cdot|$ is the entrywise absolute value and $\mathbf{1}$ is the matrix of all ones. The results we obtained did not depend in a significant way on the choice of perturbed Jacobian since the $A_n + F_n$ are perturbations of the identity. The results we report on in Table 6.2 were obtained using the `diag` approximation of the Jacobian. We include results for tolerances $\mathtt{TOL} = 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}$ over the intervals $[0, T]$ for $T = 1$, a single period, $T = 10$, and $T = 100$. In this case N is the number of time steps necessary to satisfy the local error tolerance, TOL, over the given interval. We were not able to satisfy $h < 1/2$ to apply the Newton–Kantorovich theorem for $\mathtt{TOL} = 10^{-4}$ and $\mathtt{TOL} = 10^{-5}$ when $T = 10$ or $T = 100$. For this problem, the computed Lyapunov exponents are approximately

$$\lambda_1 = 1.88E0, \;\; \lambda_2 = 1.24E0, \;\; \lambda_3 = 6.84E-1, \;\; \lambda_4 = -8.95E-1,$$
$$\lambda_5 = -1.47E0, \;\; \lambda_6 = -2.04E0.$$

The computed Lyapunov exponents are distinct and relatively well separated which suggests some degree of integral separation in the system. The results in Table 6.2 show the componentwise bounds obtained for different tolerances and time intervals. We report on the range of bounds obtained for both the off-diagonal and the diagonal elements of Q. Note that the bounds do not depend significantly on the length of the time interval.

7. Conclusions. Under the structural assumption of integral separation we develop an error analysis for the QR factorization of a potentially infinite product of matrices. Employing a Newton–Kantorovich-type theorem, we obtain both norm bounds and componentwise bounds on the orthogonal factor and the upper triangular factor. Improvements to the bounds are possible numerically by employing a better approximation to the Jacobian.

The results here also apply with minimal modification to sequence of invertible complex valued matrices $\{A_k\}_{k=0}^{\infty}$. Integral separation is characterized through the diagonals of the upper triangular matrices $\{R_k\}_{k=0}^{\infty}$ which still have real, positive diagonal elements. The nonintegrally separated case as was considered in section 4 of [9] would be an interesting extension. The results here are easily modified to apply to the "adjoint" formulation of the discrete QR process $Q_{n+1}R_n^{-T} = A_n^{-T}Q_n$. Finally, we note the recent work on stability spectrum for differential algebraic equations [16] and for noninvertible systems of linear difference equations [2] and the possibility of developing a quantitative perturbation theory based upon the ideas in this work.

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