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On the Perturbation of LU, Cholesky, and QR Factorizations*

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ABSTRACT

In this paper error bounds are derived for a first order expansion of the LU factorization of a perturbation of the identity. The results are applied to obtain perturbation expansions of the LU, Cholesky, and QR factorizations.

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In this paper error bounds are derived for a first order expansion of the LU factorization of a perturbation of the identity. The results are applied to obtain perturbation expansions of the LU, Cholesky, and QR factorizations.

1. Introduction

Let A be of order n, and suppose that the leading principal submatrices of A are nonsingular. Then A has an LU factorization

$$A = LU, \tag{1.1}$$

where L is lower triangular U is upper triangular. The factorization is not unique; however, any other LU factorization must have the form

$$A = (LD)(D^{-1}U),$$

where D is a nonsingular diagonal matrix. Thus, if the diagonal elements of L (or U) are specified, the factorization is uniquely determined.

The purpose of this note is to establish a first order perturbation expansion for the LU factorization of A along with bounds on the second order terms. At least three authors have considered the perturbation of LU, Cholesky, and QR factorizations [1, 2, 4]. The chief difference between their papers and this one is that the former treat perturbations bounds for the decompositions in question, while here we treat the accuracy of a perturbation expansion.

Throughout this note $\|\cdot\|$ will denote a family of absolute, consistent matrix norms; i.e.,

$$|A| \le |B| \implies \|A\| \le \|B\|,$$

and

$$\|AB\| \le \|A\|\|B\|$$

whenever the product AB is defined. Thus the bounds of this paper will hold for the Frobenius norm, the 1-norm, and the ∞ norm, but not for the 2-norm (for more on these norms see [3]).

2. Perturbation of the Identity

The heart of this note is the observation that the LU factorization of the matrix $I+F$, where F is small, has a simple perturbation expansion. Specifically, write

$$F = F_{\mathrm{L}} + F_{\mathrm{U}},$$

where F_{L} is strictly lower triangular and F_{U} is upper triangular. Then

$$(I+F_{\mathrm{L}})(I+F_{\mathrm{U}}) = I + F_{\mathrm{L}} + F_{\mathrm{U}} + F_{\mathrm{L}}F_{\mathrm{U}} = I + F + O(\|F\|^2), \tag{2.1}$$

and the product of the unit lower triangular matrix $I+F_{\mathrm{L}}$ and the upper triangular matrix $I+F_{\mathrm{U}}$ reproduces $I+F$ up to terms of order $\|F\|^2$. The following theorem shows that we can move these lower order terms to the right-hand side of (2.1) to get an LU factorization of $I+F$.

Theorem 2.1. *If*

$$\|F\| \le \frac{1}{4}$$

then there is a strictly lower triangular matrix G_{L} *and an upper triangular matrix* G_{U} *satisfying*

$$\|G_{\mathrm{L}} + G_{\mathrm{U}}\| \le \frac{\|F\|^2}{1 - 2\|F\| + \sqrt{1 - 4\|F\|}}$$

such that

$$(I + F_{\mathrm{L}} + G_{\mathrm{L}})(I + F_{\mathrm{U}} + G_{\mathrm{U}}) = I + F. \tag{2.2}$$

Proof. From (2.2) it follows that the perturbations G_{L} and G_{U} must satisfy

$$G_{\mathrm{L}} + G_{\mathrm{U}} = -(F_{\mathrm{L}}F_{\mathrm{U}} + F_{\mathrm{L}}G_{\mathrm{U}} + G_{\mathrm{L}}F_{\mathrm{U}} + G_{\mathrm{L}}G_{\mathrm{U}}).$$

Starting with $G_{\mathrm{L}}^0 = 0$ and $G_{\mathrm{U}}^0 = 0$, generate strictly lower triangular and upper triangular iterates according to the formula

$$G_{\mathrm{L}}^{k+1} + G_{\mathrm{U}}^{k+1} = -(F_{\mathrm{L}}F_{\mathrm{U}} + F_{\mathrm{L}}G_{\mathrm{L}}^k + G_{\mathrm{U}}^kF_{\mathrm{U}} + G_{\mathrm{L}}^kG_{\mathrm{U}}^k). \tag{2.3}$$

Because $\|\cdot\|$ is absolute,

$$\|G_{\mathrm{L}}^k\|, \|G_{\mathrm{U}}^k\| \le \|G_{\mathrm{L}}^k + G_{\mathrm{U}}^k\|.$$

Hence if we set $\phi = \|F\|$, $\gamma_0 = 0$, and define the sequence $\{\gamma_k\}$ by

$$\gamma_{k+1} = \phi^2 + 2\phi\gamma_k + \gamma_k^2, \qquad k = 0, 1, \ldots, \tag{2.4}$$

then $\|G_{\rm L}^k + G_{\rm U}^k\| \le \gamma_k$.

Now by graphing the right hand side of (2.4), it is easy to see that if $\phi \le \frac{1}{4}$ then the sequence γ_k converges monotonically to

$$\gamma_* = \frac{\phi^2}{1 - 2\phi + \sqrt{1 - 4\phi}},$$

which is therefore an upper bound on $\|G_{\rm L}^k + G_{\rm U}^k\|$ for all k. It remains only to show that the sequence $G_{\rm L}^k + G_{\rm U}^k$ converges.

From (2.3) it follows that

$$\begin{aligned}(G_{\rm L}^{k+1} + G_{\rm U}^{k+1}) - (G_{\rm L}^k + G_{\rm U}^k) = F_{\rm L}(G_{\rm U}^{k-1} - G_{\rm U}^k) + (G_{\rm L}^{k-1} - G_{\rm L}^k)F_{\rm U} + \\ (G_{\rm L}^{k-1} - G_{\rm L}^k)G_{\rm U}^{k-1} + G_{\rm L}^k(G_{\rm U}^{k-1} - G_{\rm U}^k).\end{aligned}$$

Hence,

$$\|(G_{\rm L}^{k+1} + G_{\rm U}^{k+1}) - (G_{\rm L}^k + G_{\rm U}^k)\| \le 2(\phi + \gamma_*)\|(G_{\rm L}^k + G_{\rm U}^k) - (G_{\rm L}^{k-1} + G_{\rm U}^{k-1})\|.$$

If $2(\phi + \gamma_*) < 1$, which is certainly true if $\phi \le \frac{1}{4}$, then the series of differences is majorized by a geometric series, and the sequence converges. ■

There are some comments to be made on this theorem. In the first place the first order expansion is particularly simple: split F into its lower and upper triangular parts. We will take advantage of this simplicity in the next section, where we will derive perturbation expansions and asymptotic bounds for the LU, Cholesky, and QR factorization

The condition that $\|F\| \le \frac{1}{4}$ is perhaps too constraining, since the LU factorization of $I + F$ exists provided that $\|F\| < 1$. However, as $\|F\|$ approaches one, it is possible for the factors in the decomposition to grow arbitrarily, in which case the bounds on the second order terms must also grow. Thus the more restrictive condition can be seen as the price we pay for bounds that do not explode.

As $\|F\|$ goes to zero, the bound quickly assumes the asymptotic form

$$\|G_{\rm L} + G_{\rm U}\| \lesssim \|F\|^2;$$

i.e., the order constant for the second order terms is essentially one. If we write this in the form

$$\frac{\|G_{\rm L} + G_{\rm U}\|}{\|F\|} \lesssim \|F\|,$$

we see that the *relative* error in the first order expansion is of the same order as the perturbation itself, with order constant one.

Finally, Theorem 2.1 treats an LU decomposition of $I+F$ in which L is unit lower triangular. In analyzing symmetric permutations, we may want to take $L=U^{\mathrm{T}}$. In this case, we may work with slightly different matrices, illustrated below for $n=3$:

$$\hat{F}_{\mathrm{L}} = \begin{pmatrix} \frac{1}{2}f_{11} & 0 & 0 \\ f_{21} & \frac{1}{2}f_{22} & 0 \\ f_{31} & f_{32} & \frac{1}{2}f_{33} \end{pmatrix} \quad \text{and} \quad \hat{F}_{\mathrm{U}} = \begin{pmatrix} \frac{1}{2}f_{11} & f_{12} & f_{13} \\ 0 & \frac{1}{2}f_{22} & f_{23} \\ 0 & 0 & \frac{1}{2}f_{22} \end{pmatrix} \tag{2.5}$$

If $\hat{G}_{\mathrm{L}}$ and $\hat{G}_{\mathrm{U}}$ are defined analogously, the proof of Theorem 2.1 goes through *mutatis mutandis*. For these matrices a useful inequality is

$$\|\hat{F}_{\mathrm{L}}\|_{\mathrm{F}}, \|\hat{F}_{\mathrm{U}}\|_{\mathrm{F}} \le \frac{1}{\sqrt{2}}\|F\|_{\mathrm{F}}, \tag{2.6}$$

where $\|\cdot\|_{\mathrm{F}}$ denotes the Frobenius norm.

3. Applications

In this section we will apply the results of the previous section to get perturbation expansions for the LU, the Cholesky, and the QR decompositions. We will present only first order terms, since bounds for the second order terms can be derived from Theorem 2.1, and since the rate of convergence of these bounds to zero, suggests that the first order expansions will be satisfactory for all but the most delicate work. We will also derive asymptotic bounds for the first order terms.

Our first application is to the problem we began with: the perturbation of the LU decomposition. Let A have the LU decomposition (1.1) and let $\tilde{A}=A+E$. Then

$$L^{-1}\tilde{A}U^{-1} = I + L^{-1}EU^{-1} \equiv I+F.$$

Let F_{L} and F_{U} be as in the last section. Then $I+F \cong (I+F_{\mathrm{L}})(I+F_{\mathrm{U}})$ is the first order approximation to the LU factorization of $I+F$. It follows that

$$\tilde{A} \cong L(I+F_{\mathrm{L}})(I+F_{\mathrm{U}})U,$$

is the first order approximation to the LU factorization of $\tilde{A}$. Note that because F_{L} is unit lower triangular, this expansions preserves the scaling of the diagonal elements of L.

By taking norms we can derive the following asymptotic perturbation bound

$$\frac{\|\tilde{L}-L\|}{\|L\|} \lesssim \|L^{-1}\|\|U^{-1}\|\|A\|\frac{\|E\|}{\|A\|} \equiv \kappa_{\mathrm{LU}}(A)\frac{\|E\|}{\|A\|}. \tag{3.1}$$

Thus $\kappa_{\mathrm{LU}}(A) = \|L^{-1}\|\|U^{-1}\|\|A\|$ serves as a condition number for the LU decomposition of A. When A is square, this number is never less than the usual condition number $\kappa(A) = \|A\|\|A^{-1}\|$ and can be much larger. Bounds on the U factor can be derived similarly.

An unhappy aspect of the bound (3.1) is that it overestimates the perturbation of the leading part of the LU factorization. Specifically, if we partition

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{pmatrix},$$

then $A_{11} = L_{11}U_{11}$ and the condition number for this part of the factorization is $\kappa_{\mathrm{LU}}(A_{11})$, which is in general smaller than $\kappa_{\mathrm{LU}}(A)$. The perturbation in L_{21}, can then be estimated from the equation $L_{21} = A_{21}U_{11}^{-1}$.[1]

If A is symmetric and positive definite, then A has the Cholesky factorization

$$A = R^{\mathrm{T}}R,$$

where R is upper triangular. Let $\tilde{A} = A + E$, where E is symmetric. Setting, as above, $F = R^{-\mathrm{T}}ER^{-1}$ and defining $\hat{F}_{\mathrm{U}}$ as in (2.5), we have

$$\tilde{R} \cong (I + \hat{F}_{\mathrm{U}})R.$$

By (2.6) and the consistency of the 2-norm with the Frobenius norm, we have

$$\frac{\|\tilde{R} - R\|_{\mathrm{F}}}{\|R\|_2} \lesssim \frac{1}{\sqrt{2}}\|R^{-\mathrm{T}}\|_2\|R^{-1}\|_2\|E\|_{\mathrm{F}} = \frac{\kappa_2(A)}{\sqrt{2}}\frac{\|E\|_{\mathrm{F}}}{\|A\|_2}.$$

where $\kappa_2(A) = \|A\|_2\|A^{-1}\|_2$ is the usual condition number in the 2-norm.

[1] An alternative approach is to set

$$\check{L} = \begin{pmatrix} L_{11} & 0 \\ L_{21} & I \end{pmatrix}$$

so that

$$\check{L}^{-1}\begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} U_{11}^{-1} = \begin{pmatrix} I \\ 0 \end{pmatrix} \equiv J.$$

The proof of Theorem 2.1 can easily be adapted to give a bound on the perturbation of the LU factorization of a perturbation of J and hence on the perturbation of the LU factorization of $\begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix}$.

Finally, let A, now rectangular, be of full column rank, and consider the QR factorization

$$A = QR,$$

where Q has orthonormal columns and R is upper triangular with positive diagonal elements. The key to the derivation of the bounds is the equation

$$A^{\mathrm{T}}A = R^{\mathrm{T}}R;$$

i.e., R is the Cholesky factor of $A^{\mathrm{T}}A$.

As usual, let $\tilde{A} = A + E$, and let E_A be the orthogonal projection of E onto the column space of A. Then $A^{\mathrm{T}}E = A^{\mathrm{T}}E_A$. It follows that

$$\tilde{A}^{\mathrm{T}}\tilde{A} \cong A^{\mathrm{T}}A + A^{\mathrm{T}}E_A + E_A^{\mathrm{T}}A \equiv A^{\mathrm{T}}A + F.$$

Hence with $\hat{F}_{\mathrm{U}}$ as above, we have

$$\tilde{R} \cong (I + \hat{F}_{\mathrm{U}})R.$$

In particular,

$$\frac{\|\tilde{R} - R\|_{\mathrm{F}}}{\|R\|_2} \lesssim \sqrt{2}\kappa_2(A)\frac{\|E_A\|_{\mathrm{F}}}{\|A\|_2},$$

where $\kappa_2(A) = \|R\|_2\|R^{-1}\|_2$. Since $\tilde{Q} = \tilde{A}\tilde{R}^{-1}$, we have

$$\tilde{Q} \cong Q(I - \hat{F}_{\mathrm{U}}) + ER^{-1},$$

from which it follows that

$$\|\tilde{Q} - Q\|_{\mathrm{F}} \lesssim \kappa_2(A)\frac{\sqrt{2}\|E_A\|_{\mathrm{F}} + \|E\|_{\mathrm{F}}}{\|A\|_2}. \tag{3.2}$$

Asymptotically, the bounds derived in this section agree with the bounds in [1, 4], with the exception of (3.2), which is a little sharper owing to the presence of $\|E_A\|_{\mathrm{F}}$.

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