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CHECKING NONSINGULARITY OF TRIDIAGONAL MATRICES*

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Abstract. I. Bar-On, B. Codenotti, and M. Leoncini presented a linear time algorithm for checking the nonsingularity of general tridiagonal matrices [*BIT*, 36:206, 1996]. A detailed implementation of their algorithm, with some extensions to possibly reducible matrices, is further described in the present paper.

Key words. Tridiagonal Matrices, Error Analysis.

AMS subject classifications. 65F15.

1. Introduction. The solution of systems of linear equations is a common task in large scale scientific applications. An important aspect in these calculations is the ability to verify numerical reliability of the computed solution [5]. For example, suppose we want to solve the linear system $Ax = f$, and we compute a solution that is backward stable, i.e., $\hat{x}$ satisfies some slightly perturbed system $\hat{A} = \hat{x}\hat{f}$. Then, the actual (forward) error affecting $\hat{x}$ may still be arbitrarily large when A is closely singular. The closeness to being singular is therefore an important aspect to be considered when choosing the "right" algorithm to solve a linear system [9]. However, the notion of closeness to being singular requires more thought. For example, is the upper bidiagonal matrix

$$U = \begin{bmatrix} 1 & -2 & & \\ & \ddots & \ddots & \\ & & 1 & -2 \\ & & & 1 \end{bmatrix}$$

close to being singular or not? In the classical sense, the matrix is almost singular for we can change the entry $u_{n,1}$ to $-\frac{1}{2^{n-1}}$ to get a singular matrix. However, this matrix is clearly far from singular if we restrict the perturbations to its two main diagonals, which contain the only non zero elements. Thus it is important to define what is meant by this concept. In the classical nomenclature, closeness to being singular is determined by the singular values of the matrix being relatively small [7, 11]. The existence of such singular values implies that relatively small perturbations in the matrix elements would yield a singular matrix and vice versa. The computation of the singular values of the matrix is quite a standard task in today's software packages [1]. In this paper we consider the other approach to this problem, namely the closeness to singularity with respect to the non zero elements of the matrix. This problem in its generality has been shown to be NP-Hard [10]. However, for tridiagonal matrices, it was recently shown that this could be solved in linear time; see [2]. In the present work we proceed with a detailed description of this algorithm for the case

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of general tridiagonal matrices. As noted above, this is of importance for the sake of the reliability of the computed solution, and for the decision on which algorithm to choose for solving a corresponding tridiagonal system. For example, in [3, 4, 6] we present a fast tridiagonal solver for systems with totally nonsingular coefficient matrices, a property which can be verified using the algorithm we present in this paper. Formally, given a tridiagonal matrix T and a non negative tridiagonal matrix $E \geq |T|$, we define the radius of nonsingularity to be

$$\rho(T,E) = \sup \left\{ \theta \,|\, \overline{T} = T + \delta T,\ |\delta T| \leq \theta E,\ \det(\overline{T}) \neq 0 \right\}.$$

In sections 2 and 3 we give some necessary background for the problem. In section 4 we present the algorithm, and in section 5 some numerical examples are shown.

2. Notation. We denote a tridiagonal matrix T by

$$T = \begin{bmatrix} a_1 & c_2 & & \\ b_2 & a_2 & \ddots & \\ & \ddots & \ddots & c_n \\ & & b_n & a_n \end{bmatrix}, \qquad \begin{array}{l} b_1 = 0, \\ \\ c_1 = 0, \end{array}$$

and $\mathcal{T}(b_k, a_k, c_k)$. We consider the case where these coefficients are not known exactly as is usual in floating point scientific computations [5]. We can then denote the input coefficients by the set of tridiagonal matrices

$$\overline{T} = T + \delta T, \qquad |\delta T| \leq \mathcal{T}(\Delta b_k, \Delta a_k, \Delta c_k).$$

To simplify the discussion that follows we assume further that:

- No off-diagonal coefficient is exactly zero.
- The perturbations to the non zero coefficients are bounded by

  $$\hat{\theta}|(\cdot)| < \Delta(\cdot) < |(\cdot)|,$$

  with $\hat{\theta}$ the precision by which we store the coefficients in memory. For example, $\hat{\theta} \approx 10^{-16}$ in standard double precision.
- The perturbations to the non exact, but zero coefficients, are at least as large as the tiniest positive real number in the system, i.e., $\approx 10^{-300}$.

Let us define

$$\theta_k^{(b)} = \frac{\Delta b_k}{|b_k|}, \quad \theta_k^{(a)} = \frac{\Delta a_k}{|a_k|}, \quad \theta_k^{(c)} = \frac{\Delta c_k}{|c_k|},$$

for those coefficients which are non zero, and $\theta_T = \min_k(\theta_k^{(a)}, \theta_k^{(b)}, \theta_k^{(c)})$. Then,

$$\overline{T} = T + \delta T, \quad |\delta T| \leq \theta_T E, \quad E = \mathcal{T}(e_k, d_k, f_k)$$

with

$$e_k = \frac{\Delta b_k}{\theta_T}, \quad d_k = \frac{\Delta a_k}{\theta_T}, \quad f_k = \frac{\Delta c_k}{\theta_T}.$$

Note that $\hat{\theta} \leq \theta_T$ and that $E \geq |T|$. We may now define the radius of non singularity with respect to the non negative tridiagonal matrix E to be

$$\rho(T,E) = \sup \left\{ \theta \,|\, \overline{T} = T + \delta T,\ |\delta T| \leq \theta E,\ \det(\overline{T}) \neq 0 \right\}.$$

Hence, if this number is relative large the matrix is far from being singular.

3. Nonsingularity. In Figure 3.1 we present a simple algorithm for checking that a given irreducible tridiagonal matrix is nonsingular. The algorithm will work properly provided there are no rounding errors in the computation.

$d_1 = a_1,\ k = 2$
DO
  IF $d_{k-1} \neq 0$ THEN
    $d_k = a_k - \frac{b_k}{d_{k-1}} c_k$
  ELSE
    $k = k{+}1,\ d_k = a_k$
  END IF
  IF $k \geq n$ EXIT
  $k = k{+}1$
END DO
IF $(k = n \ \wedge \ d_n = 0)$ WRITE('Matrix is Singular')

FIG. 3.1. *Algorithm for checking singularity of irreducible tridiagonal matrices.*

However, as discussed in the previous section, the coefficients are usually not known exactly, and rounding errors further contribute to this problem. We therefore consider the more general question of verifying the possible nonsingularity of the matrices in

$$\overline{T} = T + \delta T, \quad |\delta T| \leq \overline{\theta} E, \quad \overline{\theta} E = \mathcal{T}(\Delta b_k, \Delta a_k, \Delta c_k), \tag{3.1}$$

for some given parameters $\overline{\theta}$ and $E \geq |T|$.

Let us denote the input coefficients by the range of closed intervals

$$\begin{bmatrix} \ddots & \mathcal{C}_k \equiv [c_k - \Delta c_k, c_k + \Delta c_k] \\ \mathcal{B}_k \equiv [b_k - \Delta b_k, b_k + \Delta b_k] & \mathcal{A}_k \equiv [a_k - \Delta a_k, a_k + \Delta a_k] \end{bmatrix} \tag{3.2}$$

and the first possible diagonal pivots $\overline{d}_1$ by the closed interval $\mathcal{D}_1 = \mathcal{A}_1$. Then, we can show that the kth diagonal pivot belongs to an extended closed interval of one of the following forms:

$$\mathcal{D} = [\alpha, \beta], \text{ or } \qquad (\alpha, \beta)^{(c)} \equiv \{x \leq \alpha, \beta \leq x\},$$

for some $-\infty < \alpha \leq \beta < \infty$, the interval $\mathcal{D} = [\infty]$, or

$$\mathcal{D} = [-\infty, \alpha] \equiv \{x \leq \alpha\}, \text{ or } \qquad [\beta, \infty] \equiv \{x \geq \beta\}.$$

Viewed differently, they correspond to regular closed intervals on a Riemann circle through the (x,z)-plane with radius $\frac{1}{2}$ and center at $(0,\frac{1}{2})$. The right half of the circle correspond to the positive real axis, and the left half to the negative one. The south pole $(0,0)$ is mapped to the origin and the north pole $(0,1)$ to infinity. In this way, we get a one-to-one correspondence with the extended real line with the above set of intervals corresponding to regular closed intervals on this circle; see [8].

In summary, instead of computing d_k we compute the set of possible values for $\overline{d}_k$ using

$$\mathcal{D}_k \quad = \quad \left\{ \begin{array}{ll} \overline{a}_k - \frac{\overline{b}_k}{\overline{d}_{k-1}}\overline{c}_k, & \begin{array}{c} \overline{b}_k \in \mathcal{B}_k, \overline{c}_k \in \mathcal{C}_k, \\ \overline{a}_k \in \mathcal{A}_k, \overline{d}_{k-1} \in \mathcal{D}_{k-1}, \end{array} \end{array} \right\},$$

where division by zero and infinity are defined appropriately; see [2]. The set of perturbed matrices (3.1) is nonsingular whenever $0 \notin \mathcal{D}_n$.

4. Code description. We describe in this section the algorithm for checking the nonsingularity of the set of interval matrices (3.1), for some given parameters $T, E, \overline{\theta}$. We assume here that $\overline{\theta} \geq 10\hat{\theta}$, where $\hat{\theta}$ is the machine precision, and denote the input coefficients as in (3.2).

We begin with an overall description of the code. To represent the diagonals of the original matrix, i.e.

$$\overline{a}_k \in \mathcal{A}_k = [a_k^{(-)}, a_k^{(+)}], \quad a_k^{(-)} = a_k - \Delta a_k, \quad a_k^{(+)} = a_k + \Delta a_k,$$

we use the two real arrays $a^{(-)}$ and $a^{(+)}$ respectively. We have two options for the interval of the product of the off-diagonal elements. When $b_k c_k$=0

$$\overline{b}_k\overline{c}_k \in [-G_k, G_k], \quad G_k = \max(\overline{b}_k\overline{c}_k), \quad \text{GZER(k)} = \text{.TRUE.} \tag{4.1}$$

The other alternative is that the product is of the same sign, i.e.

$$\text{GPOS(k)} = \left\{ \begin{array}{ll} \text{.TRUE.} & \text{if } b_k c_k > 0, \\ \text{.FALSE.} & \text{if } b_k c_k < 0. \end{array} \right. \tag{4.2}$$

Here, $|\overline{b}_k\overline{c}_k| \in [g_k, G_k]$ for

$$g_k = (|b_k| - \Delta b_k)(|c_k| - \Delta c_k), \qquad G_k = (|b_k| + \Delta b_k)(|c_k| + \Delta c_k). \tag{4.3}$$

Then, to describe the extended closed intervals that span the possible values for the pivots $\overline{d}_k \in \mathcal{D}_k$, we use the following logical arrays together with the two real arrays $d^{(-)}$ and $d^{(+)}$. We let

$$\text{PZER(k)=.TRUE.} \quad \text{represent} \quad \mathcal{D}_k = [0],$$

and then

$$\left. \begin{array}{c} \text{PNFY(k)=.TRUE.} \\ \text{LNFY(k)=.TRUE.,} \ d_k^{(+)} \\ d_k^{(-)}, \ \text{RNFY(k)=.TRUE.} \end{array} \right\} \quad \text{represent} \quad \left\{ \begin{array}{l} \mathcal{D}_k = [\infty], \\ \mathcal{D}_k = [-\infty, d_k^{(+)}], \\ \mathcal{D}_k = [d_k^{(-)}, \infty]. \end{array} \right.$$

Lastly, we let

$$\left.\begin{array}{l}\text{INCL(k)=.TRUE.}\\ \text{INCL(k)=.FALSE.}\end{array}\right\} \quad \text{denote} \quad \left\{\begin{array}{l}\mathcal{D}_k = [d_k^{(-)}, d_k^{(+)}],\\ \mathcal{D}_k = (d_k^{(-)}, d_k^{(+)})^{(c)}.\end{array}\right.$$

We also use SNG(k)=.TRUE. to note that the kth leading submatrix may become singular, i.e., $0 \in \mathcal{D}_k$. This may be of interest for some other applications; see [3, 6]. We now proceed to compute $\overline{d}_k$ as follows:
For $k = 1$ we let

PZER(k)=.TRUE. in case $\overline{a}_k \equiv 0$.

Otherwise, $\mathcal{D}_k = [a_k^{(-)}, a_k^{(+)}]$ with INCL(k)=.TRUE.

Then, SNG(k)=.TRUE. in case $0 \in \mathcal{D}_k$.

We set PNFY(k), LNFY(k), RNFY(k) to .FALSE.

Then, for $k = 2, \ldots, n$ we proceed iteratively as follows (leaving out some details such as setting INCL(k), etc.).

4.1. The simple cases. The first simple case is when $\mathcal{D}_{k-1} = [0]$, that is when PZER(k-1)=.TRUE. Here, either GZER(k)=.TRUE., see (4.1), and then the matrix could clearly become singular. Otherwise, we get $\mathcal{D}_k = [\infty]$ so PNFY(k) is set to .TRUE. This leads us to the second simple case which is $\mathcal{D}_{k-1} = [\infty]$. Clearly, here, we can apply the same steps as we did for k=1 above.

4.2. The case of a regular closed interval. This is when INCL(k-1)=.TRUE. so that $\mathcal{D}_{k-1}$ is one of the following.

1. Totally negative $[-M_{k-1}, -m_{k-1}]$, or totally positive $[m_{k-1}, M_{k-1}]$.
2. Totally nonpositive $[-M_{k-1}, 0]$ or totally nonnegative $[0, M_{k-1}]$.
3. Both positive and negative $[-L_{k-1}, M_{k-1}]$.

To construct $\mathcal{D}_k$ we assume first that GZER(k)=.FALSE.

1. For GPOS(k) as defined in (4.2), let

$$\text{(4.4)}\quad \text{POS} = ((d_{k-1}^{(+)} < 0) \ \wedge \ \neg\text{GPOS(k)}) \vee (\text{GPOS(k)} \ \wedge \ (0 < d_{k-1}^{(-)})).$$

Then,

$$\overline{d}_k = \left\{\begin{array}{ll}\overline{a}_k - |\frac{\overline{b}_k \overline{c}_k}{\overline{d}_{k-1}}|, & \text{if POS},\\ \overline{a}_k + |\frac{\overline{b}_k \overline{c}_k}{\overline{d}_{k-1}}|, & \text{if } \neg\text{POS}.\end{array}\right.$$

We can then use g_k, G_k as defined in (4.3) to conclude that

$$\text{(4.5)}\qquad \mathcal{D}_k = \left\{\begin{array}{ll}[a_k^{(-)} - \frac{G_k}{m_{k-1}}, a_k^{(+)} - \frac{g_k}{M_{k-1}}], & \text{if POS},\\ [a_k^{(-)} + \frac{g_k}{M_{k-1}}, a_k^{(+)} + \frac{G_k}{m_{k-1}}], & \text{if } \neg\text{POS}.\end{array}\right.$$

2. Similarly, let

$$\text{(4.6)}\quad \text{POS} = ((d_{k-1}^{(+)} = 0) \ \wedge \ \neg\text{GPOS(k)}) \vee (\text{GPOS(k)} \ \wedge \ (0 = d_{k-1}^{(-)})).$$

Then,

$$\mathcal{D}_k = \begin{cases} [-\infty, a_k^{(+)} - \frac{g_k}{M_{k-1}}], & \text{if POS,} \\ [a_k^{(-)} + \frac{g_k}{M_{k-1}}, \infty], & \text{if } \neg\text{POS,} \end{cases} \tag{4.7}$$

follows from (4.5) above.

3. Finally, we deduce that

$$\mathcal{D}_{k-1} = [-L_{k-1}, 0] \ \cup \ [0, M_{k-1}],$$

and therefore can apply the previous result. Then,

$$\mathcal{D}_k = \begin{cases} [-\infty, a_k^{(+)} - \frac{g_k}{L_{k-1}}] \ \cup \ [a_k^{(-)} + \frac{g_k}{M_{k-1}}, \infty] & \text{if } \neg\text{GPOS,} \\ [a_k^{(-)} + \frac{g_k}{L_{k-1}}, \infty] \ \cup \ [-\infty, a_k^{(+)} - \frac{g_k}{M_{k-1}}] & \text{if GPOS,} \end{cases}$$

and

$$\mathcal{D}_k = \begin{cases} (a_k^{(+)} - \frac{g_k}{L_{k-1}}, a_k^{(-)} + \frac{g_k}{M_{k-1}})^{(c)}, & \text{if } \neg\text{GPOS,} \\ (a_k^{(+)} - \frac{g_k}{M_{k-1}}, a_k^{(-)} + \frac{g_k}{L_{k-1}})^{(c)}, & \text{if GPOS,} \end{cases} \tag{4.8}$$

with INCL(k)=.FALSE.

For GZER(k)=.TRUE. we get similarly

$$\mathcal{D}_k = [a_k^{(-)} - \frac{G_k}{m_{k-1}}, a_k^{(+)} + \frac{G_k}{m_{k-1}}],$$

for case (1) above, and otherwise the whole line.

4.3. The case of an interval with one end at infinity. As in the previous section, we now have that LNFY(k-1) or RNFY(k-1) are .TRUE. so that the interval $\mathcal{D}_{k-1}$ is either

1. Totally negative $[-\infty, -m_{k-1}]$, or totally positive $[m_{k-1}, \infty]$.
2. Totally nonpositive $[-\infty, 0]$, or totally nonnegative $[0, \infty]$.
3. Both positive and negative $[-\infty, m_{k-1}]$ or $[-m_{k-1}, \infty]$.

To build the interval $\mathcal{D}_k$, we follow the same steps as before. Let,

$$\text{POS} = (\ \text{LNFY(k-1)} \wedge \neg\text{GPOS(k)}\ ) \vee \ (\ \text{GPOS(k)} \wedge \text{RNFY(k-1)}\ ).$$

Then, for GZER(k)=.FALSE., we get

1. From the analysis in (4.5)

$$\mathcal{D}_k = \begin{cases} [a_k^{(-)} - \frac{G_k}{m_{k-1}}, a_k^{(+)}], & \text{if POS,} \\ [a_k^{(-)}, a_k^{(+)} + \frac{G_k}{m_{k-1}}], & \text{if } \neg\text{POS.} \end{cases} \tag{4.9}$$

2. Similarly from that in (4.7)

$$\mathcal{D}_k = \begin{cases} [-\infty, a_k^{(+)}], & \text{if POS,} \\ [a_k^{(-)}, \infty], & \text{if } \neg\text{POS.} \end{cases}$$

3. Finally, (4.8) implies

$$\mathcal{D}_k = \begin{cases} (a_k^{(+)}, a_k^{(-)} + \frac{g_k}{m_{k-1}})^{(c)}, & \text{if POS}, \\ (a_k^{(+)} - \frac{g_k}{m_{k-1}}, a_k^{(-)})^{(c)}, & \text{if } \neg\text{POS}, \end{cases} \tag{4.10}$$

with INCL(k)=.FALSE.

Clearly, for GZER(k)=.TRUE. we get the same results as before.

4.4. The case of the complement interval. Here INCL(k-1)=.FALSE., so the interval now spans the complement to the pivot's value. Similarly, to what we did before, we now consider the corresponding open intervals that are

1. Totally negative $(-M_{k-1}, -m_{k-1})$, or totally positive (m_{k-1}, M_{k-1}).
2. Totally nonpositive $(-M_{k-1}, 0)$ or totally nonnegative $(0, M_{k-1})$.
3. Both positive and negative $(-L_{k-1}, M_{k-1})$.

We then construct $\mathcal{D}_k$, assuming first GZER(k)=.FALSE., as follows.

1. Here, since

$$\mathcal{D}_{k-1} = \begin{cases} [-\infty, -M_{k-1}] \cup [-m_{k-1}, \infty], & \text{or} \\ [-\infty, m_{k-1}] \cup [M_{k-1}, \infty], \end{cases}$$

we can use (4.9) and (4.10) with POS(k) as defined in (4.4). Hence,

$$\mathcal{D}_k = \begin{cases} [a_k^{(-)} - \frac{G_k}{M_{k-1}}, a_k^{(+)}] \cup (a_k^{(+)} - \frac{g_k}{m_{k-1}}, a_k^{(-)})^{(c)} & \text{if POS}, \\ [a_k^{(-)}, a_k^{(+)} + \frac{G_k}{M_{k-1}}] \cup (a_k^{(+)}, a_k^{(-)} + \frac{g_k}{m_{k-1}})^{(c)} & \text{if } \neg\text{POS}. \end{cases}$$

This implies more simply that

$$\mathcal{D}_k = \begin{cases} (a_k^{(+)} - \frac{g_k}{m_{k-1}}, a_k^{(-)} - \frac{G_k}{M_{k-1}})^{(c)}, & \text{if POS}, \\ (a_k^{(+)} + \frac{G_k}{M_{k-1}}, a_k^{(-)} + \frac{g_k}{m_{k-1}})^{(c)}. & \text{if } \neg\text{POS}, \end{cases} \tag{4.11}$$

with INCL(k)=.FALSE.

2. Now we can use (4.11) to conclude that

$$\mathcal{D}_k = \begin{cases} [a_k^{(-)} - \frac{G_k}{M_{k-1}}, \infty] & \text{if POS}, \\ [-\infty, a_k^{(+)} + \frac{G_k}{M_{k-1}}] & \text{if } \neg\text{POS}, \end{cases}$$

with POS as defined in (4.6).

3. Finally, we have

$$\mathcal{D}_{k-1} = [-\infty, -L_{k-1}] \cup [M_{k-1}, \infty],$$

to which we can again apply (4.9). Hence,

$$\mathcal{D}_k = \begin{cases} [a_k^{(-)} - \frac{G_k}{L_{k-1}}, a_k^{(+)}] \cup [a_k^{(-)}, a_k^{(+)} + \frac{G_k}{M_{k-1}}] & \text{if } \neg\text{GPOS}, \\ [a_k^{(-)}, a_k^{(+)} + \frac{G_k}{L_{k-1}}] \cup [a_k^{(-)} - \frac{G_k}{M_{k-1}}, a_k^{(+)}] & \text{if GPOS}, \end{cases}$$

and therefore

$$\mathcal{D}_k = \begin{cases} [a_k^{(-)} - \frac{G_k}{L_{k-1}}, a_k^{(+)} + \frac{G_k}{M_{k-1}}], & \text{if } \neg\text{GPOS}, \\ [a_k^{(-)} - \frac{G_k}{M_{k-1}}, a_k^{(+)} + \frac{G_k}{L_{k-1}}], & \text{if GPOS}. \end{cases}$$

Similarly, for GZER(k)=.TRUE. we then get, the whole line for the first two cases above (1 and 2), and

$$\mathcal{D}_k = [a_k^{(-)} - \frac{G_k}{m_{k-1}}, a_k^{(+)} + \frac{G_k}{m_{k-1}}],$$

with $m_{k-1} = \min(L_{k-1}, M_{k-1})$ for the last.

5. Numerical Examples. In this section we present some numerical examples for checking the radius of nonsingularity of tridiagonal matrices. The examples are listed in Table 5.1, numbered from 0 to 8, and the description of each is self explanatory. We used double precision, i.e. $\hat{\theta} = 2^{-53} \approx 10^{-16}$ to compute the radius of nonsingularity as

$$\rho = \sup \left\{ \theta \mid \theta = 2^i \hat{\theta},\ \overline{T} = T + \delta T,\ |\delta T| \leq \theta |T|,\ \det(\overline{T}) \neq 0 \right\}.$$

The results, depicted in Table 5.2, show that the matrix 2 is highly nonsingular whereas the matrices 4 and 6 become quickly singular as n grows.

	b	a	c
0	rand	rand	rand
1	-1	2	-1
2	1	4	1
3	-0.5	2; a(1)=1	-2
4	-1; b(2),b(n)=1	1	2
5	1	1	1
6	2	3; a(1)=1	1
7	-1	2; a(n)=1	-1
8	1; b(2)=-1	1	2

TABLE 5.1
Test Examples.

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	$n = 10$	$n = 10^2$	$n = 10^3$	$n = 10^4$
0	1.56E-02	3.91E-03	4.88E-04	1.53E-05
1	1.56E-02	1.22E-04	1.91E-06	1.49E-08
2	2.50E-01	2.50E-01	2.50E-01	2.50E-01
3	3.91E-03	6.10E-05	4.77E-07	3.73E-09
4	1.56E-02	4.44E-16	2.22E-16	2.22E-16
5	6.25E-02	3.91E-03	4.88E-04	6.10E-05
6	1.22E-04	2.22E-16	2.22E-16	2.22E-16
7	3.91E-03	6.10E-05	4.77E-07	3.73E-09
8	6.25E-02	3.91E-03	4.88E-04	1.22E-04

TABLE 5.2
Radius of Nonsingularity.

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