

A Set of Test Matrices

1. Introduction. For the testing of the adequacy and efficiency of any computing method it is clearly very desirable to have readily available a set of reliable test data. The material discussed below has been found by the author to be of great utility for this purpose. It is surmised that it may also be of interest to many others engaged in the testing of new techniques for the inversion of matrices and the determination of characteristic roots and vectors. Furthermore, the results may be of interest also for purely theoretical reasons.

The exact inverses of a sequence of ten nonsymmetric and again of ten symmetric matrices of extremely poor condition, their determinants, and their largest and smallest characteristic roots and associated vectors as well have all been calculated. These are available in the UMT file. These matrices were obtained by a simple modification of the well known Hilbert matrix, and while they share many features characteristic of that matrix, they differ from it in many other important aspects.

The data calculated also permit an examination of the closeness of certain bounds proposed by OSTROWSKI, PARKER, *et al.*

2. The sequence of matrices. The set of matrices mentioned above is obtained from the sequence of "positive" matrices.

$$A_n \equiv (a_{ij}) = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 2^{-1} & 3^{-1} & & (n+1)^{-1} \\ 3^{-1} & 4^{-1} & & (n+2)^{-1} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ n^{-1} & (n+1)^{-1} & & (2n-1)^{-1} \end{pmatrix}, \quad n = 1, 2, 3, \dots$$

Thus $a_{ij} = 1$ for all $j = 1, 2, 3, \dots$, and $a_{ij} = (i + j - 1)^{-1}$ for $i = 2, 3, \dots$; $j = 1, 2, 3, \dots$.

The matrix A_n has the following properties:

- a. The determinant d_n of A_n is of the form $(-1)^{n-1} \delta_n^{-1}$, where $\delta_n > 0$ is an integer.
- b. The elements $\alpha_{ij}^{(n)}$ of A_n^{-1} are integers. Further,

$$\sum_{i=1}^n \alpha_{ij}^{(n)} = \begin{cases} 1 & \text{for } j = 1 \\ 0 & \text{for } j \neq 1. \end{cases}$$

- c. The characteristic root of largest absolute value is positive, that of smallest absolute value negative.

The nonsymmetric matrices A_n are thus finite segments of a matrix A which is closely related to the well known symmetric Hilbert matrix

$$(2.1) \quad B = (b_{ij}), \quad b_{ij} = (i + j - 1)^{-1}$$

for $i, j = 1, 2, 3, \dots$. The matrix B has been discussed in many places, e.g., by Todd [1], and many of its properties are now known.

In giving brief sketches in substantiation of some of the properties of A_n we shall prove first that δ_n satisfies the following recursion formula:

$$(2.2) \quad \delta_{n+1} = \binom{2n}{n-1} \binom{2n}{n} (2n+1) \delta_n$$

for $n = 1, 2, 3, \dots$, with $\delta_1 = 1$.

Multiplying each column of d_{n+1} by the denominator in the last row, and then dividing outside by the product of these factors, yields

$$d_{n+1} = \frac{1}{(n+1)(n+2)\cdots(2n+1)} \begin{vmatrix} n+1 & n+2 & \cdots & 2n+1 \\ n+1 & n+2 & \cdots & 2n+1 \\ 2 & 3 & & n+2 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 1 & 1 & \cdots & 1 \end{vmatrix}.$$

The following further steps, carried out in the order indicated, lead to (2.2):

1. Subtract the last column from each of the others, making use of the fact that

$$\frac{n+j}{i+j-1} - \frac{2n+1}{n+i} = \frac{(n-i+1)(n-j+1)}{(i+j-1)(n+i)}.$$

2. Remove from the first n columns the respective factors $n, n-1, \dots, 1$ to the outside, and reduce the determinant to the order n .

3. Finally remove from all the rows except the first the respective factors

$$\frac{n-1}{n+2}, \frac{n-2}{n+3}, \dots, \frac{1}{2n},$$

getting

$$(2.3) \quad \begin{aligned} d_{n+1} &= - \frac{n!(n-1)!}{(n+1)(n+2)\cdots(2n+1)(n+2)(n+3)\cdots 2n} d_n \\ &= - \left[\frac{(n-1)!}{(n+2)\cdots(2n)} \right]^2 \cdot \frac{n}{(2n+1)(n+1)} d_n \\ &= - \binom{2n}{n-1}^{-2} \cdot \frac{n}{(2n+1)(n+1)} d_n, \end{aligned}$$

which proves (2.2).

The solution of the difference formula (2.3) leads to

$$(2.4) \quad d_n = (-1)^{n-1} \frac{[1!2! \cdots (n-2)!(n-1)!]^3}{(n-1)!(n+1)!(n+2)! \cdots (2n-1)!}$$

for $n = 1, 2, 3, \dots$.

Consequently,

$$\det A_n = (-1)^{n-1} \frac{[1!2! \cdots (n-1)!]^4}{1!2! \cdots (2n-1)!} n.$$

In [1] it was shown that for the finite segment B_n of order n of Hilbert's matrix,

$$\det B_n = \frac{[1!2! \cdots (n-1)!]^4}{1!2! \cdots (2n-1)!},$$

so that

$$\det A_n = (-1)^{n-1}n \det B_n.$$

The value of d_n may be estimated quite easily using (2.2) and Stirling's formula $n! \sim (n/e)^n(2\pi n)^{1/2}$; the result is

$$|d_n| \sim 3^n 2^{-2n(n-1)} \phi(n),$$

with $\phi(n)$ of the form $C_0 n^2$, C_0 denoting a constant.

TABLE 1a. Values of δ_n

n	
1	1
2	6
3	720
4	15 12000
5	5 33433 60000
6	31 05223 67232 00000
7	29541 55782 75110 09280 · 10 ⁴
8	45669 60589 07168 10735 · 10 ¹²
9	11430 90871 53174 41088 · 10 ²²
10	46206 89394 79146 91316 · 10 ³²

TABLE 1b. Measures of condition

n	$d(A_n)$	$M(A_n)$	$P(A_n)$
1	1	1	
2	6 ⁻¹	12	12 · 587
3	720 ⁻¹	540	354 · 51
4	(15120 · 10 ²) ⁻¹	17280	13090
5	(53343 · 10 ⁶) ⁻¹	67200 · 10 ¹	45057 · 10 ¹
6	(31052 · 10 ¹²) ⁻¹	23814 · 10 ³	15259 · 10 ³
7	(29542 · 10 ¹⁹) ⁻¹	80681 · 10 ⁴	51270 · 10 ⁴
8	(45670 · 10 ²⁷) ⁻¹	28333 · 10 ⁶	17164 · 10 ⁶
9	(11431 · 10 ³⁷) ⁻¹	95447 · 10 ⁷	57364 · 10 ⁷
10	(46207 · 10 ⁴⁷) ⁻¹	33640 · 10 ⁹	19158 · 10 ⁹

A listing of the values δ_n for $n = 1, 2, \dots, 10$, rounded to 20 significant figures, is given in Table 1a. The extremely rapid increase of δ_n is worthy of note; it serves to underline the poor "condition" of the A_n , as measured in terms of d_n . As will be shown later other, more suitable measures of condition,

$$M(A) = n \cdot \|A\| \|A^{-1}\|, \quad \|A\| = \max_{i,j} |a_{ij}|$$

$$P(A) = |\lambda_{\max}(A)/\lambda_{\min}(A)|,$$

are indicative of the same phenomenon.

Next a few remarks about the inverses A_n^{-1} . All the elements of A_n^{-1} are

integers. In fact, it can be shown that for $i = 1, 2, \dots$, we have

$$\alpha_{i1}^{(n)} = (-1)^{n-i} \binom{n+i-1}{i-1} \binom{n}{i}$$

while for $i = 2, 3, \dots$ and $j = 1, 2, \dots, n$, we have

$$\alpha_{i,j+1}^{(n)} = (-1)^{i-j} k_{i,j+1} \binom{n+i-1}{i+j} \binom{n+j}{i+j}$$

where

$$k_{i,j+1} = \binom{i+j}{j} \binom{i+j-1}{j-1} i.$$

Let us proceed to the characteristic roots λ_i and characteristic vectors x_i of A_n , arranging the λ_i according to increasing absolute value: $|\lambda_1| \leq |\lambda_2| \leq \dots \leq |\lambda_n|$; we shall set $\lambda_1 \equiv \lambda_m$, $\lambda_n \equiv \lambda_M$. Let the vector x_i have the components x_{ij} , $j = 1, 2, \dots, n$.

Since

$$\det [A - \lambda I] = (-1)^n \lambda [\lambda^{n-1} - (\sum_i a_{ii}) \lambda^{n-2} + \dots] + (-1)^{n-1} \delta_n^{-1},$$

it follows immediately that there is always at least one positive characteristic root. It seems that there is only one positive characteristic root, the others being negative.

The existence of a positive characteristic root also follows from the result of FROBENIUS [2] that the root λ_M of largest absolute value of any positive non-decomposable matrix is positive and simple, and may be associated with a proper vector having positive components only, the only vector possible that possesses this property.

Estimates for the λ_i are readily calculated from the following theorem due to PARKER [3]:

Let $U = (u_{ij})$ be an arbitrary matrix of order n . Put

$$\xi = n^{-1} \sum_{i=1}^n |u_{ii}|; \quad P_i = \sum_{j=1, j \neq i}^n |u_{ij}|, \quad Q_j = \sum_{i=1, i \neq j}^n |u_{ij}|;$$

$$S_i = P_i + |u_{ii} - \xi|, \quad S = \max_i S_i; \quad T_j = Q_j + |u_{jj} - \xi|; \quad T = \max_j T_j.$$

Then for every characteristic root λ of U

$$(2.5) \quad |\lambda - \xi| \leq \min (S, T).$$

Furthermore, the number ξ may be replaced by any other number.

Applying (2.5) to the matrix A_n , for $\xi = 0$, it is seen that the maximum column sum T is a bound:

$$(2.6) \quad \lambda_M^{(n)} < \log (n+1) + \gamma,$$

with $\gamma = 0.577 \dots$ denoting Euler's constant.

Bounds for the components of x_M may be obtained by means of Ostrowski's

theorem [4]:

Let $A_n = (a_{ij})$ be a matrix of order n of positive elements. Put

$$R_i = \sum_{j=i}^n a_{ij}, \quad i = 1, 2, \dots, n; \quad R = \max_i R_i, \quad r = \min_i R_i;$$

$$k_1 = \min_i a_{ii}, \quad k_2 = \min_{i \neq j} a_{ij}; \quad \sigma_1 = [(r - k_1)/(R - k_1)]^{1/2}.$$

Further, let the positive components x_{M_j} of the characteristic vector x_M belonging to λ_M be normalized so that

$$x_{Mn} \leq x_{M, n-1} \leq \dots \leq x_{M2} \leq x_{M1} = 1.$$

Then

$$k_2/(R - r + k_2) < x_{Mn} \leq \sigma_1$$

provided $R \neq r$.

In our case

$$R = n, \quad k_1 = (2n - 1)^{-1}, \quad k_2 = (2n - 2)^{-1}, \quad r = \sum_{j=1}^n (n + j - 1)^{-1}.$$

It is found that

$$(2.7) \quad (2n^2)^{-1}[1 + O(n^{-1})] < x_{Mn} < [\log 2/n]^{1/2}[1 + O(n^{-1})].$$

The characteristic roots of least absolute value λ_m are frequently also of interest. If the $\lambda_i^{(n)}$ are distinct, then

$$A_n^{-1} = \sum_{i=1}^n (1/\lambda_i^{(n)})x_i^{(n)} \cdot r_i^{(n)}$$

where the $x_i^{(n)}$ denote the characteristic column vectors of A_n belonging to $\lambda_i^{(n)}$, and the $r_i^{(n)}$ are the characteristic row vectors of the transposed matrix A_n^T belonging to $\lambda_i^{(n)}$. The smallest root $\lambda_m^{(n)}$ may then be found as the dominant root $\mu_M^{(n)}$ of A_n^{-1} .

If it is further known that the roots λ of the matrix $U = (u_{ij})$ are real, then (2.5) permits the conclusion

$$\lambda \geq \xi - \min(S, T);$$

if, in addition, the particular root $\lambda = \mu_M$ is negative, then clearly

$$(2.8) \quad \mu_M^{-1} \leq [\xi - \min(S, T)]^{-1}.$$

Another upper bound for λ_m is provided by the fact that for definite matrices

$$(n\|A\|)^{-1} \leq \|A^{-1}\| \leq |\lambda_m|^{-1}.$$

Thus

$$(2.9) \quad |\lambda_m| \leq \|A^{-1}\|^{-1}.$$

3. The inverses and determinants. The first ten inversions were carried out by the method of partitioning [5]. A tabulation of the inverse A_6^{-1} computed by this method is given in Table 2.

TABLE 2. *The inverse of A_6*

$$A_6^{-1} = \begin{bmatrix} -6 & 630 & -6720 & 22680 & -30240 & 13860 \\ 105 & -7350 & 88200 & -317520 & 441000 & -207900 \\ -560 & 29400 & -376320 & 1411200 & -2016000 & 970200 \\ 1260 & -52920 & 705600 & -2721600 & 3969000 & -1940400 \\ -1260 & 44100 & -604800 & 2381400 & -3528000 & 1746360 \\ 462 & -13860 & 194040 & -776160 & 1164240 & -582120 \end{bmatrix}$$

Certain interesting properties of these inverses have already been pointed out before. The following features of the A_n^{-1} are also noteworthy:

a. It is seen that

$$\text{sgn } \alpha_{ij}^{(n)} = \begin{cases} (-1)^{i+j-1} & \text{for } i \geq 1, j \geq 1, \text{ for } n \text{ even} \\ (-1)^{i+j-1} & \text{for } i \geq 1, j \geq 2, \text{ for } n \text{ odd} \\ (-1)^{i+j} & \text{for } i \geq 1, j = 1, \text{ for } n \text{ odd.} \end{cases}$$

b. $\|A_n^{-1}\| = \alpha_{k+1, k+1}^{(n)}$ or $\alpha_{k, k+1}^{(n)}$ with $k + 1 < n$ for $n > 3$.

Now

$$\|A_n^{-1}\| \geq |\alpha_{nn}^{(n)}| \sim C_1 2^{4n}.$$

Inspection of the $\|A_n^{-1}\|$ suggests that

$$(3.1) \quad \|A_n^{-1}\| \sim C_2 2^{5n} \quad \text{with } C_2 \approx 4 \cdot 10^{-3}.$$

With these estimates it is seen that the measures $M(A_n)$ are approximately

$$(3.2) \quad M(A_n) \sim C_2 n 2^{5n},$$

so that the order of ill-conditioning is about that of Hilbert's matrix.

The exact values of the $M(A_n)$ are shown in Table 1b.

It has been stated [6] that "average" matrices have M -condition numbers of the order $n^{1/2} \log n$, and P -condition numbers of the order n . In the light of such orders for condition numbers the matrices A_n must indeed be called extremely pathological.

There is a large number of techniques in matrix algebra which are specifically restricted to symmetric positive matrices H ; for the use of such procedures there have been calculated the matrices

$$H_n = A_n^T A_n.$$

From the reciprocals of A_n those of H_n are easily calculated as

$$(3.3) \quad H_n^{-1} = A_n^{-1} (A_n^{-1})^T.$$

The inverses H_n^{-1} thus also consist of integer elements only. It is known (TAUSSKY [8]) that the condition (in several senses) of AA^T is worse than that of A .

Obviously in $H_{k+1} = (h_{ij}^{(k+1)})$,

$$(3.4) \quad h_{ij}^{(k+1)} = 1 + [(i+1)(j+1)]^{-1} + [(i+2)(j+2)]^{-1} + \dots + [(i+k)(j+k)]^{-1} \\ = h_{ij}^{(k)} + [(i+k)(j+k)]^{-1}$$

for all $i, j \leq k, k = 1, 2, \dots$, with $h_{ij}^{(1)} = 1$. Consequently,

$$h_{ii}^{(k+1)} = 1 + \Psi'(i) - \sum_{j=k+1}^{\infty} (i + j)^{-2},$$

where $\Psi(x) = \Gamma'(x + 1)/\Gamma(x + 1)$. Further, for fixed k ,

$$(3.5) \quad \max_{i,j} h_{ij}^{(k)} = h_{11}^{(k)} = 1 + \Psi'(1) - \sum_{j=k}^{\infty} (1 + j)^{-2} = \pi^2/6 - \sum_{j=k}^{\infty} (i + j)^{-2}.$$

A listing of H_6 is provided in Table 3.

TABLE 3. The matrix H_6

$$H_6 = \begin{pmatrix} \frac{5369}{3600} & \frac{19}{14} & \frac{431}{336} & \frac{1867}{1512} & \frac{12107}{10080} & \frac{1\ 62997}{1\ 38600} \\ & \frac{2\ 22581}{1\ 76400} & \frac{29}{24} & \frac{169}{144} & \frac{1241}{1080} & \frac{17911}{15840} \\ & & \frac{8\ 22949}{7\ 05600} & \frac{41}{36} & \frac{403}{360} & \frac{6563}{5940} \\ & & & \frac{70\ 88041}{63\ 50400} & \frac{11}{10} & \frac{359}{330} \\ & & & & \frac{68\ 97529}{63\ 50400} & \frac{71}{66} \\ & & & & & \frac{8196\ 07009}{7683\ 98400} \end{pmatrix}$$

4. **Characteristic roots and vectors.** Since there is a unique characteristic root $\lambda_M^{(n)}$ of largest absolute value the power method [7] may be used to isolate $\lambda_M^{(n)}$, while simultaneously obtaining the associated characteristic vector $x_M^{(n)}$:

$$(4.1) \quad \begin{aligned} A_n x_{k-1}^{(n)} &= \lambda_k^{(n)} x_k^{(n)}, \quad k = 1, 2, 3, \dots \\ \lim_{k \rightarrow \infty} \lambda_k^{(n)} &= \lambda_M^{(n)}, \quad \lim_{k \rightarrow \infty} x_k^{(n)} = x_M^{(n)}, \end{aligned}$$

TABLE 4. Characteristic roots

n	$\lambda_M^{(n)}$	$\lambda_m^{(n)}$
1	1.000 000	
2	1.448 403	-.115 0693
3	1.707 105	-.481 5399 · 10 ⁻²
4	1.886 632	-.144 1324 · 10 ⁻³
5	2.022 999	-.448 9833 · 10 ⁻⁵
6	2.132 376	-.139 7499 · 10 ⁻⁶
7	2.223 362	-.433 6577 · 10 ⁻⁸
8	2.301 055	-.134 0623 · 10 ⁻⁹
9	2.368 717	-.412 9309 · 10 ⁻¹¹
10	2.428 554	-.126 7649 · 10 ⁻¹²

provided the initial arbitrary vector $x_0^{(n)}$ is not orthogonal to $x_M^{(n)}$. The rate of convergence increases with the ratio between $\lambda_M^{(n)}$ and the next characteristic root of A_n .

The absolutely largest elements of A_n occur in the first row; it is therefore advisable to normalize the $x_M^{(n)}$ by keeping its first element equal to unity. In carrying out the computation a considerable saving in labor may be further achieved by utilizing the values of $x_M^{(n)}$ obtained at the n th step to start the next step with a vector $x_0^{(n+1)}$ whose first n components were identical with $x_M^{(n)}$. Proceeding in this manner there was obtained in seven or less iterations an agreement to six decimal places in both characteristic roots and vectors.

The characteristic roots $\lambda_M^{(n)}$ are shown in the middle column of Table 4; as indicated by (2.6) they actually do not grow faster than $\log n$.

The characteristic vectors $x_M^{(n)}$ belonging to the $\lambda_M^{(n)}$ are listed in Table 5a. Their smallest components $x_{Mn}^{(n)}$ seem to decrease as n^{-1} . The bounds given in (2.7) thus seem a bit wide.

The characteristic roots $\lambda_m^{(n)} = \mu_M^{(n)}$ of least absolute value were also calculated, together with their characteristic vectors $x_m^{(n)}$, now normalized to have their last component equal to unity. The values of $\lambda_m^{(n)}$ are shown in the third column of Table 4. Here the inequality (2.8), with $\xi = 0$, is found to restrict the roots fairly well, the upper bounds— $\min(S^{(n)}, T^{(n)})^{-1}$ being, at least for $n \leq 10$, less than 30 per cent too high.

For purposes of comparison the resulting condition numbers $P(A_n)$ were also computed; they are exhibited in the last column of Table 1b. These suggest the following rough estimate:

$$(4.2) \quad P(A_n) \sim C_3 2^{5n} \log n, \quad C_3 \approx 8 \cdot 10^{-3},$$

which, with (3.2), gives,

$$(4.3) \quad P(A_n) \sim (2/n) \log n M(A_n);$$

Todd [1] found for Hilbert's matrix B

$$\pi n^{-1} M(B_n) < P(B_n) < \pi M(B_n).$$

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