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An accurate method for the LU decomposition of amazing matrices

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ABSTRACT

Amazing matrices $P_{n,b}$ arise in several important combinatorial problems. In [13], a question was raised concerning how to obtain an LU factorization of these matrices. In this work, we answer this question for the case $b = 2$ and introduce a high relative accurate algorithm to compute such a factorization. Numerical experiments are provided to demonstrate the accuracy and effectiveness of the proposed method.

1. Introduction

Let n and b be positive integers. The amazing matrix $P_{n,b} = [P(i,j)]_{i,j=0}^{n-1}$ is defined as an $n \times n$ matrix with entries

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$$P(i,j) = \frac{1}{b^n} \sum_{r \geq 0} (-1)^r \binom{n+1}{r} \binom{n-1-i+(j+1-r)b}{n}. \tag{1.1}$$

The amazing matrix arises in many interesting problems in the field of Combinatorics (cf. [5,8,12]). In particular, it is related to the carries obtained when summing n numbers base b and it is also related to the process of b-riffle shuffling n cards. Total positivity of this matrix was conjectured in [5], partially proved in [12] and finally completely proved in [13]. Recall that a matrix is totally positive (TP) if all its minors are nonnegative. TP matrices are also called totally nonnegative matrices. This class of matrices has applications in many fields: see the surveys [1,6], the classical book [9] and the recent books [7,16]. It is known (cf. Proposition 2.11 of [16]) that a nonsingular TP matrix has a unique factorization of the form LDU, where L is a unit diagonal lower triangular TP matrix, U is a unit diagonal upper triangular TP matrix and D is a diagonal matrix with positive diagonal entries. In p. 11 of [13], the authors say "A natural problem is to find out the corresponding factorization of the amazing matrix". This paper solves this problem for $b = 2$. Moreover, we provide a method to obtain $P_{n,2} = L(DU)$ with high relative accuracy.

Let us recall that an algorithm can be performed with high relative accuracy (HRA) if it does not include subtractions (except of initial data), that is, if it only includes products, divisions, sums (of numbers of the same sign) and subtractions of initial data (cf. [3,4]). HRA algorithms are very desirable in Numerical Linear Algebra, which has been achieved for some algorithms and some classes of matrices (cf. [2,14,15,10]).

The paper is organized as follows. In Section 2 we present the LU decomposition of the amazing matrix for $b = 2$ and show that it can be performed to HRA. In Section 3, we illustrate the high accuracy of our method with some numerical examples.

From now on, we shall use the following notation. The elementary matrix $E_r(\alpha) = (e_{ij})_{0 \leq i,j \leq n-1}$, $1 \leq r \leq n-1$, is the $n \times n$ matrix that has unit diagonal, α in place $(r, r-1)$ and 0 elsewhere. We will also use the notation $\prod_{i=m,\, s}^{n} e_i$, which denotes the product of the terms e_i for indices i ranging from m to n with step size s.

2. Amazing matrices

Let us recall that the amazing matrix $P_{n,b} = [P(i,j)]_{i,j=0}^{n-1}$ is given by (1.1). In the case when $b = 2$ for any n, from [8] we have the following expression for the entries of the matrix $P_{n,2}$

$$P(i,j) = \frac{1}{2^n} \binom{n+1}{2j-i+1}. \tag{2.1}$$

The following result presents an LU decomposition of the matrix $P_{n,2}$. Moreover, it will be shown that this decomposition can be performed with HRA.

Theorem 2.1. *The matrix $P_{n,2}$ can be factorized in the following form:*

$$P_{n,2} = LU$$

where

$$L = \prod_{k=0}^{n-2} \prod_{s=k+1,2}^{d(k+1)} E_s\left(\frac{2k+1}{n-k}\prod_{r=0}^{k}\frac{n+k-2r}{n+k-2r+1}\right),$$

with $d(k) := \begin{cases} n-2, & \text{if } n-k \text{ even,} \\ n-1, & \text{if } n-k \text{ odd,} \end{cases}$ *and U is the $n \times n$ upper triangular matrix whose nonzero entries are given by*

$$u_{ij} = \begin{cases} \dfrac{1}{2^n}\dbinom{n+1}{2j-i+1}\displaystyle\prod_{r=0}^{(i-1)/2}\frac{n+2r+2}{n-2r+1}\cdot\frac{2j-i-2r+1}{2j-2r+1}, & \text{if } i \text{ odd,} \\[2ex] \dfrac{1}{2^n}\dbinom{n+1}{2j-i+1}\displaystyle\prod_{r=0}^{(i-2)/2}\frac{n+2r+3}{n-2r}\cdot\frac{2j-i-2r}{2j-2r+1}, & \text{if } i \text{ even.} \end{cases} \tag{2.2}$$

Proof. First let us note that the amazing matrix is a Hurwitz matrix (see [13]). Therefore, we have that

$$P(i,j) = P(i+2s, j+s), \qquad 0 \le i,j \le n-1 \text{ and } s \ge 0 \text{ such that } i+2s, j+s \le n-1.$$

An upper triangular matrix U will be obtained by using elementary row operations from $P_{n,2}$. In order to do that, elementary matrices $E_i(\alpha)$, $1 \le i \le n-1$, will be used to track the operations.

Given $P^{(0)} := 2^n P_{n,2}$, let us prove by induction on $k \in \{0,1,\dots,n-2\}$ that the entries of the matrix

$$P^{(k+1)} = \prod_{s=d(k+1),-2}^{k+1} E_s\left(-\frac{2k+1}{n-k}\prod_{r=0}^{k}\frac{n+k-2r}{n+k-2r+1}\right)P^{(k)}, \tag{2.3}$$

are given by

$$P^{(k+1)}(k+1+2s, j+s) = \begin{cases} \dbinom{n+1}{2j-k}\displaystyle\prod_{r=0}^{k/2}\frac{n+2r+2}{n-2r+1}\cdot\frac{2j-k-2r}{2j-2r+1}, & \text{if } k+1 \text{ odd,} \\[2ex] \dbinom{n+1}{2j-k}\displaystyle\prod_{r=0}^{(k-1)/2}\frac{n+2r+3}{n-2r}\cdot\frac{2j-k-2r-1}{2j-2r+1}, & \text{if } k+1 \text{ even,} \end{cases} \tag{2.4}$$

for

$$s = 0, 1, \ldots, \frac{d(k+1) - k - 1}{2} \quad \text{and} \quad k = 0, 1, \ldots, n-2,$$

and the remaining entries coincide with those of the matrix $P^{(k)}$.

First, let us prove the cases $k = 0$ and 1. Let us subtract $\frac{P^{(0)}(1,0)}{P^{(0)}(0,0)} = \frac{1}{n+1}$ times the first row to the second row. So, the entries are computed as

$$\begin{aligned} P^{(1)}(1,j) &:= P^{(0)}(1,j) - \frac{1}{n+1} \cdot P^{(0)}(0,j) \\ &= \binom{n+1}{2j} - \frac{1}{n+1}\binom{n+1}{2j+1} = \frac{2j}{2j+1} \cdot \frac{n+2}{n+1}\binom{n+1}{2j}, \quad 0 \le j < n. \end{aligned}$$

Taking into account that $P_{n,2}$ is a Hurwitz matrix, in an analogous way, the entries $(3,1), (5,2) \ldots, (d(1), \frac{d(1)-1}{2})$ can be zeroed. This can be expressed in matrix form as

$$P^{(1)} := E_{d(1)}\left(-\frac{1}{n+1}\right) \cdots E_3\left(-\frac{1}{n+1}\right) E_1\left(-\frac{1}{n+1}\right) P^{(0)}.$$

These are the formulas (2.4) and (2.3) for $k = 0$.

Now, let us cancel the entry (2,1) of the matrix $P^{(1)}$. So, $\frac{P^{(1)}(2,1)}{P^{(1)}(1,1)} = \frac{3(n+1)}{n(n+2)}$ times the second row is subtracted to the third one:

$$\begin{aligned} P^{(2)}(2,j) &:= P^{(1)}(2,j) - \frac{3(n+1)}{n(n+2)} P^{(1)}(1,j) \\ &= \binom{n+1}{2j-1} - \frac{3(n+1)}{n(n+2)} \cdot \frac{2j(n+2)}{(2j+1)(n+1)}\binom{n+1}{2j} \\ &= \frac{2j-2}{2j+1} \cdot \frac{n+3}{n}\binom{n+1}{2j-1}, \quad 1 \le j < n. \end{aligned}$$

By the structure of the Hurwitz matrix, in this step the entries $(4,2), (6,3), \ldots, (d(2), d(2)/2)$ can also be zeroed. This can be expressed in matrix form as

$$P^{(2)} := E_{d(2)}\left(-\frac{3(n+1)}{n(n+2)}\right) \cdots E_4\left(-\frac{3(n+1)}{n(n+2)}\right) E_2\left(-\frac{3(n+1)}{n(n+2)}\right) P^{(1)},$$

which are the formulas (2.4) and (2.3) for $k = 1$.

Let us assume that the formulas (2.3) and (2.4) hold until some $k + 1 \ge 2$ even, and let us prove it for $k + 2$ and $k + 3$.

Let us subtract $\frac{2k+3}{n-k-1} \prod_{r=0}^{k+1} \frac{n+k-2r+1}{n+k-2r+2}$ times the row with index $k + 1$ to the following row:

$$\begin{aligned}P^{(k+2)}(k+2+2s,j+s) :=&P^{(k+1)}(k+2+2s,j+s)\\ &-\frac{2k+3}{n-k-1}\prod_{r=0}^{k+1}\frac{n+k-2r+1}{n+k-2r+2}P^{(k+1)}(k+1+2s,j+s).\end{aligned}$$

Since in step $k+1$ only the rows with the same parity as $k+1$ (i.e., $k+1+2s$) are modified, it follows that $P^{(k+1)}(k+2+2s,j+s) = P^{(k)}(k+2+2s,j+s) = P^{(k)}(k+2(s+1),j-1+(s+1))$. Also, by the induction step, we have that

$$\begin{aligned}P^{(k+2)}(k+2+2s,j+s) &= P^{(k)}(k+2(s+1),j-1+(s+1))\\ &\quad-\frac{2k+3}{n-k-1}\prod_{r=0}^{k+1}\frac{n+k-2r+1}{n+k-2r+2}P^{(k+1)}(k+1+2s,j+s)\\ &=\binom{n+1}{2j-k-1}\prod_{r=0}^{(k-1)/2}\frac{n+2r+2}{n-2r+1}\cdot\frac{2j-k-2r-1}{2j-2r-1}\\ &\quad-\frac{2k+3}{n-k-1}\prod_{r=0}^{k+1}\frac{n+k-2r+1}{n+k-2r+2}\binom{n+1}{2j-k}\cdot\\ &\quad\cdot\prod_{r=0}^{(k-1)/2}\frac{n+2r+3}{n-2r}\cdot\frac{2j-k-2r-1}{2j-2r+1}.\end{aligned}$$

Then, after factoring

$$\binom{n+1}{2j-k-1}\prod_{r=0}^{(k-1)/2}\frac{n+2r+2}{n-2r+1}\cdot\frac{2j-k-2r-1}{2j-2r+1},$$

and taking into account that

$$\prod_{r=0}^{(k-1)/2}\frac{n+2r+3}{n-2r}\cdot\frac{n-2r+1}{n+2r+2}=\prod_{r=0}^{k}\frac{n+k-2r+2}{n+k-2r+1},$$

it follows that

$$\begin{aligned}&P^{(k+2)}(k+2+2s,j+s) = \binom{n+1}{2j-k-1}\prod_{r=0}^{(k+1)/2}\frac{n+2r+2}{n-2r+1}\cdot\frac{2j-k-2r-1}{2j-2r+1},\\ &\qquad k+1\le j<n,\end{aligned}$$

for $s=0,1,\dots,\frac{d(k+2)-k-2}{2}$. This is (2.4) for $k+2$. This can be expressed using elementary matrices as follows

$$P^{(k+2)}=\prod_{s=d(k+2),-2}^{k+2} E_s\left(-\frac{2k+3}{n-k-1}\prod_{r=0}^{k+1}\frac{n+k-2r+1}{n+k-2r+2}\right)P^{(k+1)},$$

which coincides with (2.3), for $k+2$.

Finally, let us subtract $\frac{2k+5}{n-k-2}\prod_{r=0}^{k+2}\frac{n+k-2r+2}{n+k-2r+3}$ times the row with index $k+2$ to the following row. In a very similar process to the one made for $k+2$, it follows that

$$\begin{aligned}
P^{(k+3)}(k+3+2s,j+s) :={}& P^{(k+2)}(k+3+2s,j+s)\\
&-\frac{2k+5}{n-k-2}\prod_{r=0}^{k+2}\frac{n+k-2r+2}{n+k-2r+3}P^{(k+2)}(k+2+2s,j+s)\\
={}& P^{(k+1)}(k+1+2(s+1),j-1+(s+1))\\
&-\frac{2k+5}{n-k-2}\prod_{r=0}^{k+2}\frac{n+k-2r+2}{n+k-2r+3}P^{(k+2)}(k+2+2s,j+s)\\
={}& \binom{n+1}{2j-k-2}\prod_{r=0}^{(k-1)/2}\frac{n+2r+3}{n-2r}\cdot\frac{2j-k-2r-3}{2j-2r-1}\\
&-\frac{2k+5}{n-k-2}\prod_{r=0}^{k+2}\frac{n+k-2r+2}{n+k-2r+3}\binom{n+1}{2j-k-1}\cdot\\
&\cdot\prod_{r=0}^{(k+1)/2}\frac{n+2r+2}{n-2r+1}\cdot\frac{2j-k-2r-1}{2j-2r+1}\\
={}& \binom{n+1}{2j-k-2}\prod_{r=0}^{(k+1)/2}\frac{n+2r+3}{n-2r}\cdot\frac{2j-k-2r-3}{2j-2r+1},
\end{aligned}$$

$$k+2\le j<n,$$

for $s=0,1,\dots,\frac{d(k+3)-k-3}{2}$. This is (2.4) for $k+3$. This can be expressed using elementary matrices as follows

$$P^{(k+3)}=\prod_{s=d(k+3),-2}^{k+3} E_s\left(-\frac{2k+5}{n-k-2}\prod_{r=0}^{k+2}\frac{n+k-2r+2}{n+k-2r+3}\right)P^{(k+2)},$$

which coincides with (2.3), for $k+3$. This proves the induction of (2.3) and (2.4).

Now we can express the matrices L and U as follows

$$U:=\frac{1}{2^n}P^{(n-1)}=\prod_{k=n-2,-1}^{0}\ \prod_{s=d(k+1),-2}^{k+1} E_s\left(-\frac{2k+1}{n-k}\prod_{r=0}^{k}\frac{n+k-2r}{n+k-2r+1}\right)P_{n,2},$$

Algorithm 1 Computation of lower and upper triangular matrices L and U such that $P_{n,2} = LU$.

```
Require: $n$
Ensure: $B$ containing the $LU$ decomposition of $P_{n,2}$
  $B = eye(n)$
  for $k = 0 : n - 2$ do
    $m = \frac{2k+1}{n-k} \prod_{r=0}^{k} \frac{n+k-2r}{n+k-2r+1}$
    if (n-k-1)%2==0 then
      $r = n - 1$
    else
      $r = n$
    end if
    for s=k+2:2:r do
      $B(s, s/2 + k/2) = m$
    end for
  end for
  $B = TNExpand(B)$
  for $i = 0 : n - 1$ do
    for $j = i : \lfloor \frac{n+i}{2} \rfloor$ do
      if i% 2==1 then
        $B(i+1, j+1) = \frac{1}{2^n} \binom{n+1}{2j-i+1} \prod_{r=0}^{(i-1)/2} \frac{n+2r+2}{n-2r+1} \cdot \frac{2j-i-2r+1}{2j-2r+1}$
      else
        $B(i+1, j+1) = \frac{1}{2^n} \binom{n+1}{2j-i+1} \prod_{r=0}^{(i-2)/2} \frac{n+2r+3}{n-2r} \cdot \frac{2j-i-2r}{2j-2r+1}$
      end if
    end for
  end for
```

and from the previous formula, we deduce that $P_{n,2} = LU$, where

$$L = \prod_{k=0}^{n-2} \prod_{s=k+1,2}^{d(k+1)} E_s \left(\frac{2k+1}{n-k} \prod_{r=0}^{k} \frac{n+k-2r}{n+k-2r+1} \right),$$

and $U(i,j) = \frac{1}{2^n} P^{(n-1)}(i,j) = \frac{1}{2^n} P^{(i)}(i,j) = u_{ij}$ coincides with (2.2) and concludes the proof. $\square$

The calculation of the entries of U only involves additions, multiplications, and divisions of positive values, and that the subtractions occur only between integers. Hence, since L is a product of nonnegative elementary matrices, we can guarantee the HRA.

Corollary 2.2. *Let $P_{n,2}$ be the amazing matrix for $b = 2$, as defined in* (2.1). *Then the computation of the LU decomposition can be performed with HRA.*

3. Numerical experiments

An algorithm can be computed to HRA when it only uses products, quotients, additions of numbers of the same sign, or subtractions of initial data. The proof of Theorem 2.1 provides an LU factorization of the amazing matrix $P_{n,2}$, and Corollary 2.2 states that it can be computed to HRA. Algorithm 1 provides the pseudocode of such an algorithm.

Algorithm 1 with HRA has been implemented in Matlab in a function `AmazingLU`.

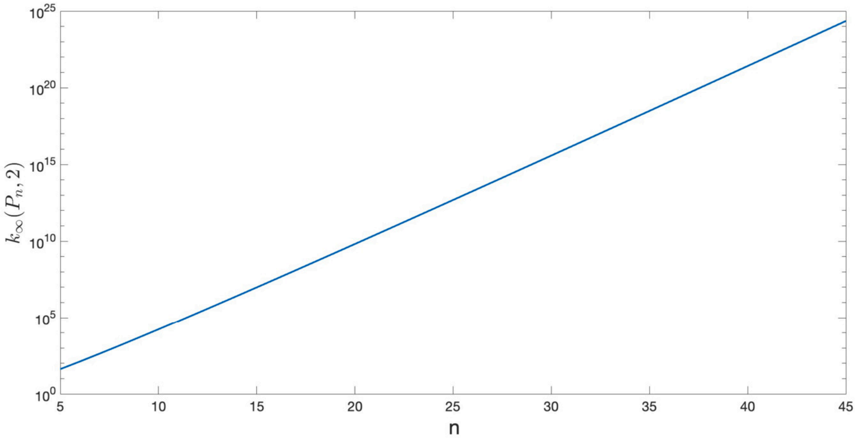

Fig. 1. Conditioning of the matrices $P_{n,2}$ for $n = 5, 6, \ldots, 45$.

Table 1
Relative errors for the LU factorization of $P_{n,2}$.

n	AmazingLU		TNBD and TNExpand	
	Mean	Max	Mean	Max
5	7.404863e-17	2.293248e-16	3.900552e-17	2.220446e-16
10	1.262962e-16	3.853791e-16	1.398899e-16	1.332268e-15
15	1.416767e-16	7.590509e-16	7.150826e-16	9.325873e-15
20	1.869995e-16	8.033617e-16	1.568052e-14	3.563816e-13
25	1.653381e-16	1.277551e-15	2.131359e-13	8.991030e-12
30	1.474159e-16	7.346573e-16	1.195425e-11	4.888255e-10
35	2.210693e-16	1.075670e-15	1.198716e-10	4.619791e-09
40	4.307734e-16	1.941909e-15	1.919285e-09	5.537288e-08
45	6.974467e-16	4.142034e-15	7.552424e-08	2.534832e-06

In order to illustrate the HRA of the LU factorization provided by the proposed algorithm, the amazing matrices $P_{n,2}$, $n = 5, 6, \ldots, 45$, have been considered. These matrices are very poorly conditioned, as it can be observed in Fig. 1.

The LU factorization of the matrices $P_{n,2}$, $n = 5, 10, 15, \ldots, 45$, has been computed with Matlab in two different ways. The first one, with HRA using the function `AmazingLU` corresponding to Algorithm 1. The second one, using the functions `TNBD` and `TNExpand` of the software library TNTool ([11]), but without HRA. The exact LU factorization has been obtained with Mathematica. Then, the componentwise relative errors for both approximations obtained with Matlab have been computed. Then, the corresponding mean and maximum relative errors have been calculated. The results can be seen in Table 1.

Finally, the determinants of the matrices $P_{n,2}$, $n = 5, 6, \ldots, 45$, have been computed with Matlab in two different ways. The first one, using the usual Matlab function `det`. The second one, as the product of the diagonal entries of the matrix U corresponding to the LU factorization obtained by Algorithm 1. This last computation is carried out with HRA. Then, the relative errors of the approximations to the determinant have

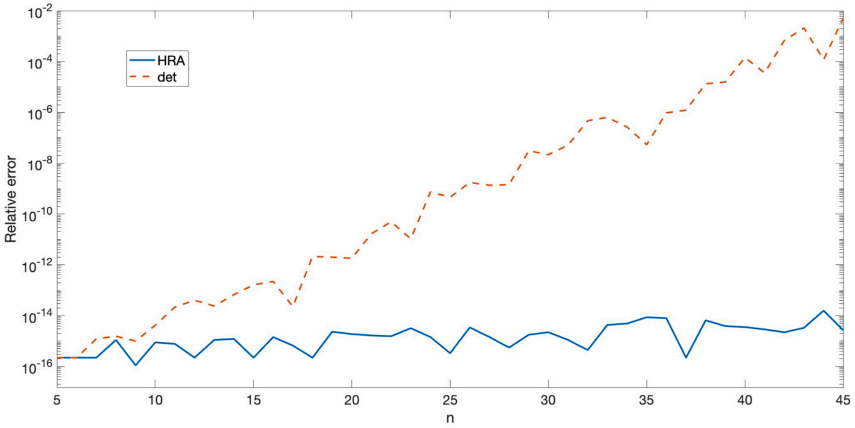

Fig. 2. Relative errors when computing $det(P_{n,2})$ for $n = 5, 6, \dots, 45$.

been calculated obtaining their exact values with Mathematica. Comparisons of these relative errors can be seen in Fig. 2. It can be observed that the approximations to the determinants obtained with the HRA approach outperform these obtained with function `det` from a point of view of accuracy.

Declaration of competing interest

The authors declare that they have no competing interests.

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Data availability

No data was used for the research described in the article.

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