Some connections between M-matrices and totally positive matrices

J.M. Peña*

University of Zaragoza, Spain

Definition. A real matrix is a **P-matrix** if all its principal minors are positive

Some classes of P-matrices:

C1: Symmetric positive definite matrices.

A matrix is totally positive if all its minors are nonnegative.
C2: Nonsingular totally positive matrices.

A nonsingular matrix A with positive diagonal elements and nonpositive off-diagonal elements is an M-matrix if $A^{-1} \geq 0$.
C3: Nonsingular M-matrices.

C4: Matrices with positive diagonal elements which are strictly diagonal dominant by rows.

C5: Matrices with positive row sums and all its off-diagonal elements bounded above by the corresponding row means (B-matrices).

Principal submatrices inherit these properties.

Generalized diagonal dominance

The **comparison matrix** $\tilde{M} = (\tilde{m}_{ij})_{1\le i,j\le n}$ of a matrix $M = (m_{ij})_{1\le i,j\le n}$ is given by $\tilde{m}_{ii} := |m_{ii}|$ and $\tilde{m}_{ij} := -|m_{ij}|$, $i = 1, \ldots, n$ and $j \neq i$.

We say that a matrix is an ***H*-matrix** if its comparison matrix is a nonsingular M-matrix.

An H-matrix with positive diagonal entries is a P-matrix.

Theorem. A is an H-matrix if and only if there exists a diagonal matrix X such that AX is strictly diagonally dominant.

The **linear complementarity problem** (LCP) consists of finding vectors $x \in \mathbf{R}^n$ satisfying

$$Mx + q \geq 0, \quad x \geq 0, \quad x^T(Mx + q) = 0, \tag{1}$$

where M is an $n \times n$ real matrix and $q \in \mathbf{R}^n$. We denote this problem by $\mathrm{LCP}(M, q)$ and its solutions by x^*.

The LCP has a **unique solution** if and only if M is a P-matrix.

If **M in (1) is a P-matrix**, then for any $x \in \mathbf{R}^n$:

$$\|x - x^*\|_\infty \leq \max_{d \in [0,1]^n} \|(I - D + DM)^{-1}\|_\infty \|r(x)\|_\infty,$$

where I is the $n \times n$ identity matrix, D the diagonal matrix $D = \mathrm{diag}(d_i)$ with $0 \leq d_i \leq 1$ for all $i = 1, \ldots, n$, x^* is the solution of the $\mathrm{LCP}(M, q)$ and $r(x) := \min(x, Mx + q)$, where the min operator denotes the componentwise minimum of two vectors.

If M in (1) is an H-matrix with positive diagonals, then

$$\max_{d\in[0,1]^n} \|(I-D+DM)^{-1}\|_\infty \le \|\tilde{M}^{-1}\max(\Lambda, I)\|_\infty, \qquad (2)$$

where $\tilde{M}$ is the comparison matrix of M, Λ is the diagonal part of M ($\Lambda := \mathrm{diag}(m_{ii})$) and $\max(\Lambda, I) := \mathrm{diag}(\max\{m_{11}, 1\}, \ldots, \max\{m_{nn}, 1\})$.

M. García-Esnaola and J.M. P., *A comparison of error bounds for linear complementarity problems of H-matrices*. Linear Algebra and its Applications 433 (2010), 956–964.

Theorem. Let us assume that $M = (m_{ij})_{1\le i,j\le n}$ is an **H-matrix with positive diagonal entries**. Let $\bar{D} = \mathrm{diag}(\bar{d}_1, \ldots, \bar{d}_n), \bar{d}_i > 0$, for all $i = 1, \ldots, n$, be a diagonal matrix such that $M\bar{D}$ is strictly diagonally dominant by rows. For any $i = 1, \ldots, n$, let $\bar{\beta}_i := m_{ii}\bar{d}_i - \sum_{j\ne i} |m_{ij}|\bar{d}_j$. Then

$$\max_{d\in[0,1]^n} \|(I-D+DM)^{-1}\|_\infty \le \max\{\frac{\max_i\{\bar{d}_i\}}{\min_i\{\bar{\beta}_i\}}, \frac{\max_i\{\bar{d}_i\}}{\min_i\{\bar{d}_i\}}\}. \qquad (3)$$

With a particular choice of $\bar{D}$, then $\bar{\beta}_i = 1$ for all i in previous theorem:

$$\max_{d\in[0,1]^n} \|(I - D + DM)^{-1}\|_\infty \leq \max\{\max_i\{\bar{d}_i\}, \frac{\max_i\{\bar{d}_i\}}{\min_i\{\bar{d}_i\}}\}. \tag{4}$$

Example. Let $k > 2$ and $M = \begin{pmatrix} 2k & -k+1 \\ -2k+2 & k \end{pmatrix}$. Then for that choice, we have $\bar{d} = (1/2, 1)^T$ and so, the bound (4) is 2. On the other hand,

$$\tilde{M} = M, \tilde{M}^{-1} = \begin{pmatrix} \frac{k}{4k-2} & \frac{k-1}{4k-2} \\ \frac{k-1}{2k-1} & \frac{k}{2k-1} \end{pmatrix} \quad \|\tilde{M}^{-1}\max(\Lambda, I)\|_\infty = \frac{3k^2 - 2k}{2k-1}.$$

Therefore the bound (2) can be arbitrarily large.

Error bounds for LCP with some subclasses of H-matrices

M. García-Esnaola and J.M. P., Error bounds for the linear complementarity problem with a Σ-SDD matrix (2013). *Linear Algebra and its Applications* **438**, pp. 1339-1346.

M. García-Esnaola and J.M. P., Error bounds for linear complementarity problems of Nekrasov matrices (2014). *Numerical Algorithms* **67**, pp. 655-667.

ORERA H., P. J.M.: Infinity norm bounds for the inverse of Nekrasov matrices using scaling matrices (2019). *Applied Mathematics and Computation* **358**, pp. 119-127.

Error bounds for LCP with P-matrices that are not H-matrices

-With **B-matrices and their generalizations**:

M. García-Esnaola and J.M. P., Error bounds for linear complementarity problems of **B-matrices** (2009). *Applied Mathematics Letters* **22**, 1071-1075.

P.-F. Dai, Error bounds for linear complementarity problems of **DB-matrices** (2011). *Linear Algebra Appl.* **434**, 830-840.

M. García-Esnaola and J.M. P., Error bounds for linear complementarity problems of **B^S-matrices** (2012). *Applied Mathematics Letters* **25**, 1379-1383.

P.-F.Dai, Ch.-J. Lu and Y.-T. Li, New error bounds for the linear complementarity problem with an **SB-matrix** (2013). *Numer. Algor.* **64**, 741-757.

M. García-Esnaola and J.M. P., **B-Nekrasov** matrices and error bounds for linear complementarity problems (2016). *Numerical Algorithms* **72**, 435-445.

More general nonsingularity conditions (**B_π^R-matrices**) have been applied to the linear complementarity problem:

NEUMANN M., P. J.M., PRYPOROVA O.: "Some Classes of Nonsingular Matrices and Applications" (2013). *Linear Algebra and its Applications* **438**, pp. 1936-1945.

GARCIA-ESNAOLA M., P. J.M.: "B_π^R-matrices and error bounds for linear complementarity problems" (2017). *Calcolo* **54**, pp. 813-822.

GARCIA-ESNAOLA M., P. J.M.: "On the asymptotic optimality of error bounds for some linear complementarity problems" (2019). *Numerical Algorithms* **80**, pp. 521-532.

ORERA H., P. J.M.: "Error bounds for linear complementarity problems of B_π^R-matrices" (2021). *Computational and Applied Mathematics* **40**: Paper 94 (13 pp.).

The class of B_π^R-matrices has also been extended to define a new class of tensors. Tensors (also called **hypermatrices**) provide a very useful tool for the treatment of Big Data:

ORERA H., P. J.M.: "B_π^R-tensors" (2019). *Linear Algebra and its Applications* **581**, pp. 247-259.

ORERA H., P. J.M.: "Beta-matrices and beta-tensors" (2022). *Filomat* **36**, pp. 4331-4338.

The class of C-matrices has also been extended to define a new class of tensors: **C-tensors**.

PANIGRAHY K., MISHRA D., P. J.M.: "On C-tensor and its application to eigenvalue localization" (2022). *Linear and Multilinear Algebra* **70**, pp. 6279-6296.

LCP and STP matrices

A matrix is *strictly totally positive* (STP) if all its minors are positive

P.N. Choudhury: Characterizing total positivity: single vector tests via linear complementarity, sign non-reversal and variation diminution. Bull. Lond. Math. Soc. 54 (2022), 791-811.

THEOREM. An $m \times n$ matrix is STP iff for every square submatrix A_r of size $r \leq m, n$, LCP(A_r, q) has a unique solution for all $q \in \mathbf{R}^r$

Inverses

J.M. P.: “M-matrices whose inverses are totally positive” (1995). *Linear Algebra and its Applications* **221**, pp. 189-194.

THEOREM. Let A be a nonsingular $n \times n$ M-matrix . Then A^{-1} is TP iff A is a tridiagonal matrix.

Characterizations of tridiagonal nonsingular M-matrices whose inverse matrix is also tridiagonal in:

A. BARRERAS, J.M. P.: “Tridiagonal M-matrices whose inverse is tridiagonal and related pentadiagonal matrices” (2019). *RACSAM* **113**, pp. 3785-3793.

Effects of finite precision arithmetic on numerical algorithms:

- Roundoff errors.
- Data uncertainty.

Key concepts:

- *Conditioning*: it measures the sensibility of solutions to perturbations of data.
- *Growth factor*: it measures the relative size of the intermediate computed numbers with respect to the initial coefficients or to the final solution.
- *Backward error*: if the computed solution is the exact solution of a perturbated problem, it measures such perturbation.
- *Forward error*: it measures the distance between the exact solution and the computed solution.

(Forward error) $\leq$ *(Backward error)* $\times$ *(Condition)*

N.J. Higham. *Accuracy and Stability of Numerical Algorithms, second ed.*. SIAM, Philadelphia, PA, 2002.

Given $a \in \mathbf{R}$, the computed element in floating point arithmetic will be denoted by either $\mathrm{fl}(a)$ or by $\hat{a}$.

Models:

$$\mathrm{fl}(a \,\mathrm{op}\, b) = (a \,\mathrm{op}\, b)(1+\delta), \quad |\delta| \leq u,$$

$$\mathrm{fl}(a \,\mathrm{op}\, b) = \frac{(a \,\mathrm{op}\, b)}{(1+\varepsilon)}, \quad |\varepsilon| \leq u,$$

with u the unit roundoff and *op* any of the elementary operations $+$, $-$, $\times$, $/$.

Given $k \in \mathbf{N}_0$ such that $ku < 1$, let us define

$$\gamma_k := \frac{ku}{1-ku}$$

We shall deal with quantities θ_k satisfying that their absolute value is upperly bounded by γ_k.

Gaussian elimination transforms a given linear system $Ax = b$ into an equivalent upper triangular linear system $Ux = c$. Briefly described, for nonsingular matrices A, it consists of a succession of $n-1$ steps resulting in a sequence of matrices as follows:

$$A = A^{(1)} \to A^{(2)} \to \cdots \to A^{(n)} = U.$$

At the end of step $t-1$, the matrix $A^{(t)}$ will have been constructed, having zeros below its main diagonal on its first $t-1$ columns:

$$A^{(t)} = \begin{pmatrix} a_{11}^{(t)} & a_{12}^{(t)} & \dots & \dots & \dots & \dots & a_{1n}^{(t)} \\ 0 & a_{22}^{(t)} & \dots & \dots & \dots & \dots & a_{2n}^{(t)} \\ \vdots & 0 & \ddots & & & & \vdots \\ \vdots & \vdots & & \ddots & & & \vdots \\ \vdots & \vdots & & & a_{tt}^{(t)} & \dots & a_{tn}^{(t)} \\ \vdots & \vdots & & & \vdots & & \vdots \\ 0 & 0 & \dots & \dots & a_{nt}^{(t)} & \dots & a_{nn}^{(t)} \end{pmatrix}.$$

To obtain $A^{(t+1)}$ from $A^{(t)}$ we produce zeros in column t below the *pivot element* $a_{tt}^{(t)}$ by subtracting multiples of row t from the rows beneath it. Rows $1, 2, \ldots, t$ are not altered, according to the formula

$$a_{ij}^{(t+1)} = \begin{cases} a_{ij}^{(t)} & \text{if } i \leq t \\ a_{ij}^{(t)} - \frac{a_{it}^{(t)}}{a_{tt}^{(t)}} a_{tj}^{(t)} & i \geq t+1,\ j \geq t+1 \\ 0 & \text{otherwise.} \end{cases}$$

The same transformations should be carried out in the vector b:

$$b = b^{(1)} \to b^{(2)} \to \cdots \to b^{(n)} = c.$$

GE with a given pivoting strategy:

$$A^{(1)} \to \tilde{A}^{(1)} \to A^{(2)} \to \tilde{A}^{(2)} \to \cdots \to A^{(n)} = U$$

The matrix $\tilde{A}^{(t)} = (\tilde{a}_{ij}^{(t)})_{1 \leq i,j \leq n}$ is obtained from the matrix $A^{(t)}$ by reordering the rows and/or columns $t, t+1, \ldots, n$ of $A^{(t)}$ according to the given pivoting strategy and satisfying $\tilde{a}_{tt}^{(t)} \neq 0$.

Growth factor

$$\rho_n^W(A) := \frac{\max_{i,j,k} |a_{ij}^{(k)}|}{\max_{i,j} |a_{ij}|}$$

ρ_n^W associated with partial pivoting of an $n \times n$ matrix is bounded above by 2^n. ρ_n^W associated with complete pivoting of an $n \times n$ matrix is "usually" bounded above by n.

Gauss elimination of a symmetric positive definite matrix (without row or column exchanges) presents $\rho_n^W = 1$.

Amodio and Mazzia have introduced the growth factor

$$\rho_n(A) := \frac{\max_k \|A^{(k)}\|_\infty}{\|A\|_\infty}.$$

P. Amodio, F. Mazzia: A new approach to backward error analysis of LU factorization, BIT 39 (1999) pp. 385–402.

Condition number

$$\kappa(A) := \|A\|_\infty \, \|A^{-1}\|_\infty.$$

The Skeel condition number:

$$\mathrm{Cond}(A) := \|\, |A^{-1}|\, |A|\, \|_\infty.$$

- $\mathrm{Cond}(A) \le \kappa(A)$
- $\mathrm{Cond}(DA) = \mathrm{Cond}(A)$ for any nonsingular diagonal matrix D

Diagonal dominance

THEOREM. (Wilkinson) If A is a nonsingular matrix diagonally dominant by rows or columns, then we can perform Gauss elimination without row exchanges, the obtained matrices $A^{(k)}[k,\ldots,n]$ preserve the same propertyfor all $k \in \{1,\ldots,n\}$ and the growth factor is $\rho_n^W(A) \leq 2$.

J.M. P.: Pivoting strategies leading to diagonal dominance by rows, *Numer. Math.* **81** (1998), pp. 293–304.

THEOREM. If the LU decomposition of a nonsingular matrix A satisfies that U is diagonally dominant by rows, then $\rho_n(A) \leq 1$ and $\mathrm{Cond}(U) \leq 2n-1$.

J.M. P.: Scaled pivots and scaled partial pivoting strategies, *SIAM J. Numer. Anal.* **41** (2003), pp. 1022-1031.

THEOREM. Let $U = (u_{ij})_{1\leq i,j\leq n}$ be an upper triangular matrix which is strictly diagonally dominant by rows and let $p := \min_{1\leq i\leq n}\{|u_{ii}|/\sum_{j=i}^{n}|u_{ij}|\}$. Then $\mathrm{Cond}(U) \leq 1/(2p-1)$.

J.M. P.: Strict diagonal dominance and optimal bounds for the Skeel condition number. *SIAM J. Numer. Anal.* **45** (2007), pp. 1107-1108.

M-matrices

Nonsingular M-matrices are matrices with nonpositive off-diagonal elements and nonnegative inverse.

An M-matrix has a row such that the diagonal element is diagonally dominant. The corresponding symmetric pivoting strategy is called **symmetric diagonally dominant** (d. d.). The computational cost can be performed $\mathcal{O}(n^2)$.

Given $Ax = b$, let $e := (1, \ldots, 1)^T$ and $b_1 := Ae$. The symmetric m.a.d.d. pivoting strategy produces the sequence of matrices

$$A = A^{(1)} \to \tilde{A}^{(1)} \to A^{(2)} \to \tilde{A}^{(2)} \to \cdots \to A^{(n)} = U$$

and the corresponding sequence of vectors

$$b_1 = b_1^{(1)} \to \tilde{b_1}^{(1)} \to b_1^{(2)} \to \tilde{b_1}^{(2)} \to \cdots \to b_1^{(n)} = c.$$

The largest component of $b_1^{(k)}[k, \ldots, n]$ determines the kth pivot.

GE with any symmetric pivoting strategy, then all matrices $A^{(t)}$ are also M-matrices.

Tests

Checking if an $n \times n$ matrix is a P-matrix requires $\mathcal{O}(2^n)$ elementary operations.

"A recursive test for P-matrices" (M. J. Tsatsomeros and L. Li). *BIT* **40** (2000), pp. 410–414.

However, checking if a matrix belongs to one subclass of P-matrices can require a low computational cost.

Examples: matrices strictly diagonally dominant by rows and with positive diagonal elements, symmetric positive definite matrices (in this case, the growth factor of checking the positivity of Gauss elimination is 1).

- **A stable test to check if a matrix is nonsingular M-matrix.**

A stable test of $\mathcal{O}(n^3)$ elementary operations to check if a matrix is a nonsingular M-matrix has been derived in:

J.M. P.: A stable test to check if a matrix is a nonsingular M-matrix. *Mathematics of Computation* **73** (2004), pp. 1385-1392.

Applications:

(1) A nonnegative square matrix B satisfies $\rho(B) < 1$ if and only if $I - B$ is a nonsingular M-matrix.

(2) If a square matrix B satisfies that $I - |B|$ is a nonsingular M-matrix, then $\rho(B) < 1$.

(3) A square Z-matrix B is positive stable (i.e., its eigenvalues have positive real parts) if and only if B is a nonsingular M-matrix.

A matrix is a *Z-matrix* if all its off-diagonal entries are nonpositive.

Theorem. *Let A be an $n \times n$ $(n \geq 3)$ nonsingular M-matrix. Let ρ_n^W be the growth factor associated with symmetric d.d. pivoting strategy. Then*

$$\rho_n^W < n - 1.$$

If we solve $Ax = b$ by Gaussian elimination with this pivoting strategy in finite precision floating point arithmetic, then the computed solution $\hat{x}$ satisfies $(A + \Delta A)\hat{x} = b$ with:

$$\|\Delta A\|_\infty < 4(n-1)\gamma_n \|A\|_\infty + O(u^2).$$

J.M. P.: A note on a paper by P. Amodio and F. Mazzia, BIT 41 (2001), pp. 640–643: $\rho_n(A) = 1$

Any symmetric d.d. pivoting strategy leads to an upper triangular matrix U which is strictly diagonally dominant by rows. Then

$$\mathrm{Cond}(U) \leq (1/(2p-1)).$$

- **A stable test to check if a matrix is STP or TP.**

A matrix is *strictly totally positive* (STP) if all its minors are positive and it is *totally positive* (TP) if all its minors are nonnegative.

Applications of the test to C.A.G.D.

M. Gasca, J.M. P.: Total positivity and Neville elimination. *Linear Algebra Appl.* **165** (1992), 25-44.

Neville elimination (NE)

If A is a nonsingular matrix of order n, it consists of $n-1$ steps:

$$A = A^{(1)} \to A^{(2)} \to \ldots \to A^{(n)} = U,$$

$$A^{(t)} = \begin{pmatrix} a_{11}^{(t)} & a_{12}^{(t)} & \ldots & \ldots & \ldots & \ldots & a_{1n}^{(t)} \\ 0 & a_{22}^{(t)} & \ldots & \ldots & \ldots & \ldots & a_{2n}^{(t)} \\ \vdots & 0 & \ddots & & & & \vdots \\ \vdots & \vdots & & \ddots & & & \vdots \\ \vdots & \vdots & & & a_{tt}^{(t)} & \ldots & a_{tn}^{(t)} \\ \vdots & \vdots & & & \vdots & & \vdots \\ 0 & 0 & \ldots & \ldots & a_{nt}^{(t)} & \ldots & a_{nn}^{(t)} \end{pmatrix}.$$

$$a_{ij}^{(t+1)} = \begin{cases} a_{ij}^{(t)} & i \le t \\ a_{ij}^{(t)} - \frac{a_{it}^{(t)}}{a_{i-1,t}^{(t)}} a_{i-1,j}^{(t)} & i \ge t+1,\ a_{i-1,t}^{(t)} \ne 0 \\ a_{ij}^{(t)} & i \ge t+1,\ a_{i-1,t}^{(t)} = 0 \end{cases}$$

The element

$$p_{ij} := a_{ij}^{(j)}, \quad 1 \le j \le i \le n,$$

is called (i,j) *pivot* of the NE of A.

The *complete Neville elimination* (CNE) of A: NE of A until obtaining U and NE of $V := U^T$.

TESTS

Growth factor:

$$\rho := \max\{\frac{\max_{i,j,k}|a_{ij}^{(k)}|}{\max_{i,j}|a_{ij}|}, \frac{\max_{i,j,k}|v_{ij}^{(k)}|}{\max_{i,j}|a_{ij}|}\}(\geq 1)$$

Theorem.

(i) *A matrix $A = (a_{ij})_{1\leq i\leq n}^{1\leq j\leq m}$ is STP if and only if we can perform the CNE of A without row or column exchanges and, for all $k = 1, \ldots, r = \min\{n, m\}$, $a_{ij}^{(k)} > 0$ for all $i, j \geq k$ and $v_{ij}^{(k)} > 0$ for all i, j with $i \geq j \geq k$.*

(ii) *The test suggested by (i) to check if A is STP can be performed in $\mathcal{O}(s^3)$ ($s = \max\{n, m\}$) elementary operations.*

(iii) *The growth factor is $\rho = 1$.*

Theorem.

(i) A square matrix $A = (a_{ij})_{1\le i,j\le n}$ is nonsingular and TP if and only if we can perform the CNE of A without row or column exchanges, the diagonal pivots are positive and, for all $k = 1, \dots, n$, $a_{ij}^{(k)} \ge 0$ for all $i, j \ge k$ and $v_{ij}^{(k)} > 0$ for all i, j with $i \ge j \ge k$.

(ii) The test suggested by (i) to check the total positivity of A can be performed in $\mathcal{O}(n^3)$ elementary operations.

(iii) The growth factor is $\rho = 1$.

J.M. P.: "Tests for the recognition of total positivity" (2013). *SeMA Journal* **62**, pp. 61-73.

Accurate algorithm: the relative error is bounded by $\mathcal{O}(\varepsilon)$, where ε is the machine precision. They are called **HRA** (with High Relative Accuracy) algorithms.

Admissible operations in algorithms with high relative precision: products, quotients, sums of numbers of the same sign and sums/subtractions of exact data. They are called **NIC** (no inaccurate cancellation) algorithms:

The only **forbidden** operation is true subtraction, due to possible cancellation in leading digits.

J. Demmel, I. Dumitriu, O. Holtz, P. Koev: Accurate and efficient expression evaluation and linear algebra, *Acta Numer.* **17** (2008), 87-145.

Evaluating $x + y + z$ is **not possible with HRA**.

For some **structured** classes of matrices, HRA algorithms can be found. But we also know that this is not possible for other classes of structured matrices. For instance, the **determinant of a Toeplitz** matrix **cannot be evaluated with HRA**.

$$B = \begin{pmatrix} a_0 & a_1 & a_2 & a_3 & a_4 \\ a_{-1} & a_0 & a_1 & a_2 & a_3 \\ a_{-2} & a_{-1} & a_0 & a_1 & a_2 \\ a_{-3} & a_{-2} & a_{-1} & a_0 & a_1 \\ a_{-4} & a_{-3} & a_{-2} & a_{-1} & a_0 \end{pmatrix}$$

Even if HRA algorithms exist, if the matrices are ill-conditioned, then they may need to be **re-parameterized**: first task to construct algorithms with HRA.

With these new parameters, new algorithms can be designed to compute the desired values (eigenvalues, singular values, inverses or solutions of the corresponding linear systems) with HRA.

In order to guarantee accurate computations for some special classes of matrices, it is crucial to find an **adequate parametrization** adapted to the special classes of matrices:

- For **diagonally dominant** M-matrices (with off-diagonal nonpositive entries and positive row sums): the off-diagonal entries and the row sums.
- For nonsingular **totally positive** (TP) matrices (with nonnegative minors): the multipliers of its Neville elimination (which correspond to their bidiagonal factorization).

HRA with TP and STP matrices

Definition. A matrix is *strictly totally positive* (STP) if all its minors are positive and it is *totally positive* (TP) if all its minors are nonnegative. They are also called totally positive and totally nonnegative, respectively.

K is TP and nonsingular **if and only if**

$$K = L_{n-1} L_{n-2} \cdots L_1 D U_1 \cdots U_{n-2} U_{n-1},$$

where the matrices L_i (resp., U_i) are nonnegative lower (resp., upper) triangular **bidiagonal** with unit diagonal and D is a **diagonal** matrix with **positive** diagonals.

Uniqueness of the factorization, under certain conditions, in:

M. Gasca, J.M. P.: A matricial description of Neville elimination with applications to total positivity. *Linear Alg. Appl.* **202** (1994), 33–54.

Theorem. *Let A be a* **nonsingular TP** *matrix. Then A admits factorizations in the form*

$$A = F_n F_{n-1} \cdots F_1 D G_1 \cdots G_n,$$

where F_i and G_i, $i \in \{1, \ldots, n\}$, are the lower and upper triangular bidiagonal matrices given by

$$F_i = \begin{pmatrix} 1 & & & & & & & \\ 0 & 1 & & & & & & \\ & \ddots & \ddots & & & & & \\ & & 0 & 1 & & & & \\ & & & m_{i0} & 1 & & & \\ & & & & m_{i+1,1} & 1 & & \\ & & & & & \ddots & \ddots & \\ & & & & & & m_{n,n-i} & 1 \end{pmatrix},$$

$$G_i^T = \begin{pmatrix} 1 &&&&&&& \\ 0 & 1 &&&&&& \\ & \ddots & \ddots &&&&& \\ && 0 & 1 &&&& \\ &&& -\widetilde{m}_{i,i-1} & 1 &&& \\ &&&& -\widetilde{m}_{i+1,i-1} & 1 && \\ &&&&& \ddots & \ddots & \\ &&&&&& -\widetilde{m}_{n,i-1} & 1 \end{pmatrix},$$

and D the diagonal matrix $diag(p_{00}, p_{11} \ldots, p_{nn})$. The entries m_{ij}, $\widetilde{m}_{ij}$ are the multipliers of the Neville elimination of A and A^T, respectively, and the entries p_{ii} are the diagonal pivots of A.

Neville elimination (NE) produces zeros in each column by adding to each row an adequate multiple of the previous one (instead of a multiple of the pivot row as in Gauss elimination).:

M. Gasca, J.M. P.: Total positivity and Neville elimination. *Linear Algebra Appl.* **165** (1992), 25-44.

The pivots of the NE of A are given by

$$p_{ij} = \frac{\det A[i-j+1,\ldots,i+1|1,\ldots,j+1]}{\det A[i-j+1,\ldots,i|1,\ldots,j]}, \quad 0 < j \leq i \leq n.$$

The multipliers of the NE of A are given by

$$m_{ij} := p_{ij}/p_{i-1,j}, \quad 1 \leq j \leq i \leq n.$$

The multipliers of the NE of A^T are given by

$$\widetilde{m}_{ij} := \widetilde{p}_{ij}/\widetilde{p}_{i-1,j}, \quad 1 \leq j \leq i \leq n,$$

where $\widetilde{p}_{ij}$ is the (i,j) pivot of A^T.

Therefore, **computing initial minors with HRA** assures to compute the bidiagonalization with HRA.

A compact notation

Given a nonsingular TP matrix $A = (a_{ij})_{1\le i,j\le n}$, a compact matrix notation $\mathcal{BD}(A)$ for the bidiagonal decomposition is given by:

$$(\mathcal{BD}(A))_{ij} = \begin{cases} m_{ij}, & \text{if } \ i > j, \\ \widetilde{m}_{ji}, & \text{if } \ i < j, \\ p_{ii}, & \text{if } \ i = j. \end{cases} ,$$

that is,

$$\mathcal{BD}(A) = \begin{pmatrix} p_{11} & \widetilde{m}_{21} & \cdots & \cdots & \widetilde{m}_{n1} \\ m_{21} & p_{22} & \widetilde{m}_{32} & \cdots & \widetilde{m}_{n2} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ m_{n-1,1} & \cdots & m_{n-1,n-2} & p_{n-1,n-1} & \widetilde{m}_{n,n-1} \\ m_{n1} & \cdots & \cdots & m_{n,n-1} & p_{nn} \end{pmatrix}.$$

Subclasses of TP matrices with accurate computations

For some **subclasses** of nonsingular totally positive matrices, the bidiagonal decomposition can be assured to high relative accuracy and so, many **accurate computations** can be also assured:

- **inverses**
- **SVD**
- **eigenvalues**
- **solution of some linear systems** ($Ax = b$, b with alternating consecutive signs).

P. Koev: Accurate computations with totally nonnegative matrices, *SIAM J. Matrix Anal. Appl.* **29** (2007), no. 3, 731–751.

- **TP matrices in Combinatorics**

A **Pascal matrix** of order n is the symmetric matrix $P = (p_{ij})_{1\leq i,j\leq n}$ with

$$p_{ij} := \binom{i+j-2}{j-1}; \quad \mathcal{BD}(P) = \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix}.$$

ALONSO P., DELGADO J., GALLEGO R., P. J.M. : Conditioning and accurate computations with Pascal matrices, *Journal of Computational and Applied Mathematics* **252** (2013), 21-26.
DELGADO J., ORERA H., P. J.M.: "Accurate Bidiagonal Decomposition and Computations with Generalized Pascal Matrices" (2021). *Journal of Computational and Applied Mathematics* **391**: Paper 113443 (10 pp.).

Jacobi-Stirling matrices formed by the Jacobi-Stirling numbers of the first and second kind, respectively.
DELGADO J., P. J.M. : Fast and accurate algorithms for Jacobi-Stirling matrices, *Applied Mathematics and Computation* **236** (2014), 253-259.

- **Generalized Vandermonde matrices**

J. Demmel and P. Koev: The Accurate and Efficient Solution of a Totally Positive Generalized Vandermonde Linear System, *SIAM J. Matrix Anal. Appl.* **27** (2005), 142-152.

- **Cauchy-Vandermonde matrices**

A. Marco, J.J. Martínez, J.M. P.: Accurate bidiagonal decomposition of totally positive Cauchy-Vandermonde matrices and applications (2017). *Linear Algebra and its Applications* **517**, 63-84.

A matrix

$$A = \begin{pmatrix} \frac{1}{x_1-d_1} & \cdots & \frac{1}{x_1-d_l} & 1 & x_1 & \cdots & x_1^{n-l-1} \\ \frac{1}{x_2-d_1} & \cdots & \frac{1}{x_2-d_l} & 1 & x_2 & \cdots & x_2^{n-l-1} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{x_n-d_1} & \cdots & \frac{1}{x_n-d_l} & 1 & x_n & \cdots & x_n^{n-l-1} \end{pmatrix}$$

is called a **Cauchy-Vandermonde matrix** for the nodes $\{x_i\}_{1\le i\le n}$ and the poles $\{d_j\}_{1\le j\le l}$ because if $l=0$ it is a classical Vandermonde matrix and if $l=n$ it is a classical Cauchy matrix (example: a **Hilbert matrix**).

- **Bernstein-Vandermonde matrices and TP matrices in C.A.G.D.**

The **Bernstein** basis is the normalized B-basis of the space of polynomials of degree less than or equal to n on a compact interval $[a, b]$:

$$b_i(t) := \binom{n}{i} \left(\frac{t-a}{b-a}\right)^i \left(\frac{b-t}{b-a}\right)^{n-i}, \quad i = 0, \ldots, n.$$

A. Marco, J.J. Martínez: A fast and accurate algorithm for solving Bernstein-Vandermonde linear systems, *Linear Algebra Appl.* **422** (2007), 616-628.

A. Marco, J.J. Martínez: Accurate computations with **Said-Ball-Vandermonde** matrices, *Linear Algebra Appl.* **432** (2010), 2894-2908.

A. Marco, J.J. Martínez: Polynomial least squares fitting in the Bernstein basis, *Linear Algebra Appl.* 433 (2010), 1254-1264.

- **Other TP matrices in C.A.G.D.**

With q-Bernstein basis:

J. Delgado, J.M. P.: Accurate computations with collocation matrices of q-Bernstein polynomials, *SIAM Journal on Matrix Analysis and its Applications* **36** (2015), 880-893.

With Lupaş basis:

J. Delgado, J.M. P.: Accurate computations with Lupaş matrices. *Applied Mathematics and Computation* **303** (2017), 171-177.

With h-Bernstein basis:

A. Marco, J. J. Martínez, R. Viaña, Accurate bidiagonal decomposition of totally positive h-Bernstein-Vandermonde matrices and applications, Linear Algebra and its Applications **579** 320-335 (2019).

With some general classes of bases used in CAGD:

E. Mainar, J.M. P.: Accurate computations with collocation matrices of a general class of bases (2018), *Numerical Linear Algebra with Applications* **25**: e2184 (12 pp.).

E. Mainar, J.M. P., B. Rubio: “Accurate bidiagonal decomposition of collocation matrices of weighted φ-transformed systems” (2020). *Numerical Linear Algebra with Applications* **27**: e2295 (16 pp.).

Rational model in CAGD: Given a normalized system of nonnegative functions $(u_0, \ldots, u_n)$ and given positive weights $w_0, \ldots, w_n$ we may consider the **rational basis**

$$\left(\frac{w_0 u_0}{\sum_{i=0}^{n} w_i u_i}, \ldots, \frac{w_n u_n}{\sum_{i=0}^{n} w_i u_i} \right) \tag{1}$$

Rational bases derived from the Bernstein and Said-Ball bases:

J. Delgado, J.M. P.: Accurate computations with collocation matrices of rational bases, *Applied Mathematics and Computation* **219** (2013), 4354-4364.

- **TP matrices in Finance**

With Schoenmakers-Coffey matrices:

J. Delgado, G. Peña, J.M. P.: Accurate and fast computations with positive extended Schoenmakers-Coffey matrices, *Numerical Linear Algebra with Applications* **23** (2016), 1023-1031.

- **Laguerre matrices**

The **generalized Laguerre polynomials** are given by

$$L_n^{(\alpha)}(t) = \sum_{k=0}^{n} (-1)^k \binom{n+\alpha}{n-k} \frac{t^k}{k!}, \quad n = 0, 1, 2, \ldots$$

They are orthogonal polynomials on $[0, \infty)$ with respect to the weight function $x^\alpha e^{-x}$ (with $\alpha = 0$: the classical Laguerre polynomials).

Laguerre matrices: $M := \left(L_{j-1}^{(\alpha)}(t_{i-1}) \right)_{1 \le i,j \le n+1}$ is the collocation matrix of the generalized Laguerre polynomials at $(0 >) t_0 > t_1 > \ldots > t_n$.

Theorem. The Laguerre matrices M are **STP** and $\mathcal{BD}(M)$ can be performed with HRA.

DELGADO J., ORERA H., P. J.M.: "Accurate computations with Laguerre matrices" (2019). *Numerical Linear Algebra with Applications* **26**: e2217 (10 pp.).

- **Bessel matrices**

The **Bessel polynomials** are given by

$$B_n(x) = \sum_{k=0}^{n} \frac{(n+k)!}{2^k (n-k)!k!} x^k, \quad n = 0, 1, 2 \ldots,$$

Given a sequence of parameters $0 < t_0 < t_1 < \cdots < t_{n-1}$, we call the collocation matrix M of the Bessel polynomials $(B_0, \ldots, B_{n-1})$ at that sequence, **Bessel matrix**.

Theorem. The Bessel matrices M are **STP** and $\mathcal{BD}(M)$ can be performed with HRA.

DELGADO J., ORERA H., P. J.M.: "Accurate algorithms for Bessel matrices" (2019). *Journal of Scientific Computing* **80**, pp. 1264-1278.

- **Wronskian matrices**

Of the **monomial** basis of polynomials and of the basis of **exponential polynomials**:

MAINAR E., P. J.M., RUBIO, B.: "Accurate computations with Wronskian matrices" (2021). *Calcolo* **58**: Paper 1 (15 pp.).

Of the **Bessel and Laguerre** polynomials:

MAINAR E., P. J.M, RUBIO, B.: "Accurate computations with Wronskian matrices of Bessel and Laguerre polynomials (2022). *Linear Algebra and its Applications* **647**, pp. 31-46.

Of the **Bernstein** and related bases:

MAINAR E., P. J.M, RUBIO, B.: "Accurate and efficient computations with Wronskian matrices of Bernstein and related bases" (2022). *Numerical Linear Algebra with Applications* **29**: e2423 (18 pp.).

- **Matrices of q-integers**

DELGADO J., ORERA H., P. J.M.: "High relative accuracy with matrices of q-integers" (2021). *Numerical Linear Algebra with Applications* **28**: e2383.

- **Collocation and Wronskian matrices of Jacobi polynomials**

MAINAR E., P. J.M, RUBIO, B.: "Accurate computations with collocation and Wronskian matrices of Jacobi polynomials" (2021). *Journal of Scientific Computing* **87**: Paper 77 (30 pp.).

- **Gramian matrices**

MAINAR E., P. J.M, RUBIO, B.: "Total positivity and accurate computations with Gram matrices of Bernstein bases" (2022). *Numerical Algorithms* **91**, pp. 841-859.

MAINAR E., P. J.M, RUBIO, B.: "Accurate computations with matrices related to bases $\{t^i e^{\lambda t}\}$" (2022). *Advances in Computational Mathematics* **48**: Paper 38 (25 pp.).

MAINAR E., P. J.M, RUBIO, B.: "Accurate computations with Gram and Wronskian matrices of geometric and Poisson bases" (2022). *RACSAM* **116**: Paper 126 (22 pp.).

- **Tridiagonal Toeplitz matrices**

DELGADO J., ORERA H., P. J.M.: "Characterizations and accurate computations for tridiagonal Toeplitz matrices" (2022). *Linear and Multilinear Algebra* **70**, pp. 4508-4527.

- **Special matrices related to gamma and beta functions**

DELGADO J., P. J.M.: "High relative accuracy with some special matrices related to gamma and beta functions". To appear in *Numerical Linear Algebra with Applications*.

- **Singular** TP matrices.

DELGADO J., KOEV P., MARCO A, MARTINEZ J.J., P. J.M., PERSSON P.-O., SPASOV S.: "Bidiagonal Decompositions of Vandermonde-Type Matrices of Arbitrary Rank" (2023). *Journal of Computational and Applied Mathematics* **426**: Paper 115064.

Matrix factorizations and HRA

A *rank revealing decomposition* of a matrix A is a decomposition $A = XDY^T$, where X, Y are well conditioned and D is a diagonal matrix. In that paper it is shown that if we can compute an accurate rank revealing decomposition then we also can compute (with an algorithm presented there) an accurate singular value decomposition. Obviously, an LDU-**factorization** with L, U well conditioned, is a rank revealing decomposition.

J. Demmel, M. Gu, S. Eisenstat, I. Slapnicar, K. Veselic and Z. Drmac: Computing the singular value decomposition with high relative accuracy, Linear Algebra Appl. **299** (1999), 21-80

They provided an algorithm for computing an **accurate singular value decomposition from a rank revealing decomposition** with a complexity of $\mathcal{O}(n^3)$ elementary operations.

Accurate SVDs of diagonally dominant M-matrices

Nonsingular M-matrices are matrices with nonpositive off-diagonal elements and nonnegative inverse.

J. Demmel and P.S. Koev: Accurate SVDs of weakly dominant M-matrices, *Numer. Math.* **98** (2004), pp. 99-104.

Given the off-diagonal entries and row sums, they present a method to compute accurately an LDU-decomposition of an $n \times n$ **M-matrix diagonally dominant by rows**. They use symmetric complete pivoting and so they can guarantee that one of the obtained triangular matrices is diagonally dominant and the other one has the off-diagonal elements with absolute value bounded above by the diagonal element.

J.M. P.: LDU decompositions with L and U well conditioned". *Electronic Transactions of Numerical Analysis* **18** (2004), pp. 198-208.

The m.a.d.d. pivoting strategy is used and so **both** triangular matrices are **diagonally dominant**.

With a **low** computational **cost**:

A. Barreras., J.M. P.: "Accurate and efficient LDU decompositions of diagonally dominant M-matrices" (2012). *Electronic Journal of Linear Algebra* **24**, pp. 153-167.

For **general** diagonally dominant matrices in:

Q. Ye, Computing singular values of diagonally dominant matrices to high relative accuracy, *Math. Comp.* **77** (2008), 2195-2230.

For **almost** diagonally dominant M-matrices:

A. Barreras., J.M. P.: "Accurate and efficient LDU decompositions of almost diagonally dominant Z-matrices" (2014). *BIT* **54**, pp. 343-356.

HRA for the SVD and for the solution of $Ax = b$ with $b \geq 0$

Nekrasov matrices

Given $A = (a_{ij})_{1\le i,j\le n}$ with $a_{ii} \neq 0$, for all $i = 1,\dots,n$,

$$h_1(A) := \sum_{j\neq 1} |a_{1j}|, \quad h_i(A) := \sum_{j=1}^{i-1} |a_{ij}| \frac{h_j(A)}{|a_{jj}|} + \sum_{j=i+1}^{n} |a_{ij}|, \quad i = 2,\dots,n.$$

Let $N := \{1,\dots,n\}$. We say that A is a **Nekrasov matrix** if $|a_{ii}| > h_i(A)$ for all $i \in N$.

A Nekrasov Z-matrix (i.e., with nonpositive off-diagonal entries) with positive diagonal entries is a nonsingular M-matrix (and so, a P-matrix).

The **parameters** that we shall use for an $n\times n$ Nekrasov Z-matrix $A = (a_{ij})_{1\le i,j\le n}$ with positive diagonal are the following n^2 parameters, which will be called **N-parameters**:

$$\begin{cases} a_{ij}, & i \neq j \\ \Delta_j(A) := a_{jj} - h_j(A), & j \in N \end{cases}$$

Theorem. Let $A = (a_{ij})_{1\le i,j\le n}$ be a Nekrasov Z-matrix with positive diagonal entries. If we know its N-parameters, then we can compute A^{-1} with **HRA** performing a subtraction–free algorithm of $\mathcal{O}(n^3)$ elementary operations.

ORERA H., P. J.M.: "Accurate inverses of Nekrasov Z-matrices" (2019). *Linear Algebra and its Applications* **574**, pp. 46-59.

HRA determinants for B-matrices and B-Nekrasov matrices in:

ORERA H., P. J.M.: "Accurate determinants of some classes of matrices" (2021). *Linear Algebra and its Applications* **630**, pp. 1-14.

Other applications of HRA algorithms for diagonally dominant matrices

HRA algorithms for diagonally dominant matrices can be applied to the **graph Laplacian matrices**, which are positive semidefinite symmetric diagonally dominant M-matrices with zero row sums and zero column sums.

They have important applications to chemistry, mathematical biology, information theory, quantum graphs or pattern recognition problems.