Numerical methods for some classes of matrices with applications to Statistics and Optimization

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TP and SR 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.

Definition. A matrix is called *sign-regular* (SR) if all $k \times k$ minors of A have the same sign (which may depend on k) for all k. If, in addition, all minors are nonzero, then it is called *strictly sign-regular* (SSR).

Variation diminishing properties of sign-regular matrices A: if A is a nonsingular $(n+1) \times (n+1)$ matrix, then A is sign-regular if and only if the number of changes of strict sign in the ordered sequence of components of $A\mathbf{x}$ is less than or equal to the number of changes of strict sign in the ordered sequence $(x_0, \ldots, x_n)$, for all $\mathbf{x} = (x_0, \ldots, x_n)^T \in \mathbf{R}^{n+1}$.

Proposition. Let A be a nonsingular TP matrix. Then all the eigenvalues of A are positive.

Nice properties of eigenvalues and eigenvectors of these matrices

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)*

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:

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

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

Accurate calculation: the relative error is bounded by $\mathcal{O}(\varepsilon)$, where ε is the machine precision.

Admissible operations in algorithms with high relative precision: products, quotients, sums of numbers of the same sign and sums/subtractions of exact data:

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

Definition. A system of functions $(u_0, \ldots, u_n)$ is *totally positive* (TP) if all its collocation matrices are totally positive.

TP systems of functions are interesting due to the *variation diminishing* properties of totally positive matrices

Definition. A TP basis $(u_0, \ldots, u_n)$ is *normalized totally positive* (NTP) if

$$\sum_{i=0}^{n} u_i(t) = 1, \quad \forall t \in I.$$

Collocation matrices of NTP systems are TP and stochastic

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

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

Optimal conditioning of Bernstein collocation matrices

DELGADO J., P. J.M.: “Optimal conditioning of Bernstein collocation matrices” (2009). *SIAM J. Matrix Anal. Appl.* **31**, 990-996..

DELGADO J., P. J.M.: “Running Relative Error for the Evaluation of Polynomials” (2009). *SIAM Journal on Scientific Computing* **31** , pp. 3905-3921.

Theorem. Let $(b_0, \dots, b_n)$ be the **Bernstein basis**, let $(v_0, \dots, v_n)$ be another NTP basis of P_n on $[0, 1]$, let $0 \leq t_0 < t_1 < \cdots < t_n \leq 1$ and $V := M\binom{v_0,\dots,v_n}{t_0,\dots,t_n}$ and $B := M\binom{b_0,\dots,b_n}{t_0,\dots,t_n}$. Then

$$\kappa_\infty(B) \leq \kappa_\infty(V).$$

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

Theorem. Let $(b_0, \ldots, b_n)$ be the **Bernstein basis**, let $(v_0, \ldots, v_n)$ be another TP basis of P_n on $[0, 1]$, let $0 \leq t_0 < t_1 < \cdots < t_n \leq 1$ and $V := M\begin{pmatrix} v_0, \ldots, v_n \\ t_0, \ldots, t_n \end{pmatrix}$ and $B := M\begin{pmatrix} b_0, \ldots, b_n \\ t_0, \ldots, t_n \end{pmatrix}$. Then

$$\mathrm{Cond}(B^T) \leq \mathrm{Cond}(V^T).$$

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.

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. To appear in *SIAM J. Numer. Anal.*.

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.

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 *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 has a complexity of $\mathcal{O}(n^3)$ elementary operations.

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

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.

Q. Ye: Computing Singular Values of Diagonally Dominant Matrices to High Relative Accuracy. To appear in *Math. Comp.*

Applications of bounds of the minimal eigenvalue of an M-matrix in linear progamming

M. García-Esnaola and J.M. P., *Sign consistent linear programing problems*. Optimization **58** (2009), 935–946.

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

R. Mathias and J. S. Pang, *Error bounds for the linear complementarity problem with a P-matrix*. Linear Algebra Appl. 132 (1990), 123–136.

X. Chen and S. Xiang, *Computation of error bounds for P-matrix linear complementarity problems*. Math. Program., Ser. A 106 (2006) 513–525.

X. Chen and S. Xiang, *Perturbation bounds of P-matrix linear complementarity problems*. SIAM J. Opt. 18 (2007), 1250–1265.

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The **linear complementarity problem** 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^*.

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

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

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

M. García-Esnaola and J.M. P., Comparisons of error bounds for linear complementarity problems of H-matrices. To appear in Linear Algebra Appl.

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

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

With a particular choice of $\bar{D}$, then $\bar{\beta}_i = 1$ for all i in Theorem 2.1 and so formula (2.2) becomes

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

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.

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

Bounds for the minimal eigenvalue

$$e := (1, \ldots, 1)^T, \quad r := Ae, \quad r_{\max} := \max_i \{r_i\}, \quad r_{\min} := \min_i \{r_i\}(> 0),$$

Theorem. Let $A = (a_{ij})_{1 \le i,j \le n}$ be a **Z-matrix strictly diagonally dominant by rows with positive diagonal entries**. Then A has a positive eigenvalue $\lambda_{\min}$ with minimal absolute value among all its eigenvalues, and satisfies:

$$(0 <) r_{\min} \le \lambda_{\min} \le r_{\max}.$$

Theorem. Let $A = (a_{ij})_{1\le i,j\le n}$ be a ***Z*-matrix strictly diagonally dominant by rows with positive diagonal entries**. Then:

$$\frac{1}{r_{\max}} \le \|A^{-1}\|_\infty \le \frac{1}{r_{\min}}. \tag{1}$$

Moreover, for any matrix norm $\|\cdot\|$, one has $(1/r_{\max}) \le \|A^{-1}\|$.

The upper bound of the right hand side of (1) was already provided by Varah for any Z-matrix strictly diagonally dominant by rows in

J. M. Varah, *A lower bound for the smallest singular value of a matrix*, Linear Algebra Appl. 11 (1975), 3–5

through $\tilde r_{\min}$ instead of $r_{\min}$:

$$\tilde r_{\max} := \max_i\{\tilde r_i\},\ \tilde r_{\min} := \min_i\{\tilde r_i\}(>0), \quad \tilde r_i := |a_{ii}| - \sum_{j\ne i}|a_{ij}|,\ i=1,\dots,n.$$

The lower bound of the right hand side of (1) **does not hold** for strictly diagonally dominant matrices whose entries have arbitrary sign:

$$A = \begin{pmatrix} 2 & 1 \\ -2 & 3 \end{pmatrix}, \quad A^{-1} = \begin{pmatrix} 3/8 & -1/8 \\ 1/4 & 1/4 \end{pmatrix}, \quad \|A^{-1}\|_\infty = \tfrac{1}{2}.$$

Given a nonsingular $n \times n$ M-matrix A, there exists a positive diagonal matrix D such that AD is strictly diagonally dominant by rows (with positive diagonal entries). Given the matrix AD, let $r^D := (AD)e$, where is given in (2.1), and given $r^D = (r_1^D, \ldots, r_n^D)^T$ then we can define

$$r_{\max}^D := \max_i \{r_i^D\}, \quad r_{\min}^D := \min_i \{r_i^D\} (> 0).$$

R. S. Varga, *On diagonal dominance arguments for bounding* $\|A^{-1}\|_\infty$, Linear Algebra Appl. 14 (1976), 211–217:

$$\|A^{-1}\|_\infty \leq \frac{\max_i\{\, d_i\}}{r_{\min}^D}.$$

Theorem. Let $A = (a_{ij})_{1\le i,j\le n}$ be a nonsingular M-matrix and let $D = \mathrm{diag}(d_i)$ be a positive diagonal matrix such that AD is strictly diagonally dominant by rows. Then A has a positive eigenvalue $\lambda_{\min}$ with minimal absolute value among all its eigenvalues, and satisfies:

$$(0<)\frac{r^D_{\min}}{\max_i\{d_i\}} \le \lambda_{\min} \le \frac{r^D_{\max}}{\min_i\{d_i\}}.$$

Besides, one has

$$\frac{\min_i\{d_i\}}{r^D_{\max}} \le \|A^{-1}\|_\infty \le \frac{\max_i\{\ d_i\}}{r^D_{\min}}.$$

J.M. P.: "Eigenvalue bounds for some classes of P-matrices". *Numerical Linear Algebra with Applications* **16** (2009), pp. 871-882.

Minimal eigenvalue of TP matrices

Given $i \in \{1, \ldots, n\}$ let

$$J_i := \{j \mid |j - i| \text{ is odd}\}, \quad K_i := \{j \neq i \mid |j - i| \text{ is even}\}.$$

Theorem. Let A be a nonsingular totally positive matrix, and let $\lambda_{\min}(> 0)$ be its minimal eigenvalue. Then:

$$\lambda_{\min} \geq \min_i \{a_{ii} - \sum_{j \in J_i} a_{ij}\}. \tag{1}$$

Gerschgorin Theorem applied to any real matrix $A = (a_{ij})_{1 \leq i,j \leq n}$ implies that

$$\min_i \{a_{ii} - \sum_{j \neq i} a_{ij}\} \leq \min_i \{\mathrm{Re}\lambda_i\}. \tag{2}$$

The following nonsingular matrix A is totally positive:

$$A = \begin{pmatrix} 12 & 7 & 1 \\ 0 & 6 & 1 \\ 0 & 3 & 8 \end{pmatrix}.$$

The eigenvalues of A are 12, 9 and 5. The bound given by (1) implies that $\lambda_{\min} \geq 5$ and so it **cannot be improved**. However, the lower bound for $\lambda_{\min}$ given by (2) is now $\lambda_{\min} \geq \min\{4, 5, 5\} = 4$.

J.M. P.: "Eigenvalue bounds for some classes of P-matrices". *Numerical Linear Algebra with Applications* **16** (2009), pp. 871-882.