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Lecture 10

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The Gershgorin Circle Theorem (Semyon Gershgorin, 1931)

(everywhere, we assume $n \geq 2$)

Theorem (Varga, Th. 1.11) Let A be an $n \times n$ (real or complex) matrix. Let Λ_i be the sum of the absolute values of the i -th row off-diagonal entries:

$$\Lambda_i = \sum_{\substack{j=1 \dots n \\ j \neq i}} |a_{ij}|$$

If λ is an eigenvalue of A , then there exists r , $1 \leq r \leq n$ such that λ lies on the disk defined by the circle of radius Λ_r around a_{rr} :

$$|\lambda - a_{rr}| \leq \Lambda_r.$$

Gershgorin Circle Corollaries

Corollary: Any eigenvalue of A lies in the union of the disks defined by the Gershgorin circles

$$\lambda \in \bigcup_{i=1 \dots n} \{\mu \in \mathbb{V} : |\mu - a_{ii}| \leq \Lambda_i\}$$

Corollary: The Gershgorin circle theorem allows to estimate the spectral radius $\rho(A)$:

$$\rho(A) \leq \max_{i=1 \dots n} \sum_{j=1}^n |a_{ij}| = \|A\|_{\infty},$$

$$\rho(A) \leq \max_{j=1 \dots n} \sum_{i=1}^n |a_{ij}| = \|A\|_1.$$

Proof

$$|\mu - a_{ii}| \leq \Lambda_i \quad \Rightarrow \quad |\mu| \leq \Lambda_i + |a_{ii}| = \sum_{j=1}^n |a_{ij}|$$

Furthermore, $\sigma(A) = \sigma(A^T)$.

Gershgorin circles: heat example I

$$A = \begin{pmatrix} \frac{2}{h} & -\frac{1}{h} & & & & & & & \\ -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & & & & & \\ & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & & & & \\ & & \ddots & \ddots & \ddots & & & & \\ & & & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & & \\ & & & & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & \\ & & & & & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & \\ & & & & & & -\frac{1}{h} & \frac{2}{h} & \\ & & & & & & & -\frac{1}{h} & \frac{2}{h} \end{pmatrix}$$

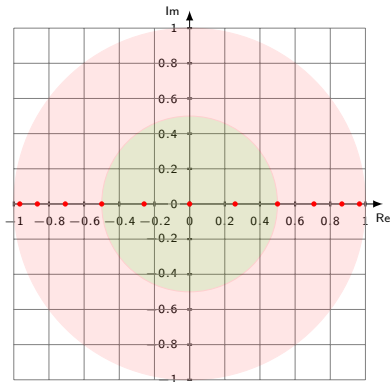
$$B = (I - D^{-1}A) = \begin{pmatrix} 0 & \frac{1}{2} & & & & & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & & & & & \\ & \frac{1}{2} & 0 & \frac{1}{2} & & & & & \\ & & \ddots & \ddots & \ddots & & & & \\ & & & \frac{1}{2} & 0 & \frac{1}{2} & & & \\ & & & & 0 & \frac{1}{2} & \frac{1}{2} & & \\ & & & & & \frac{1}{2} & 0 & \frac{1}{2} & \\ & & & & & & \frac{1}{2} & 0 & \\ & & & & & & & \frac{1}{2} & 0 \end{pmatrix}$$

We have $b_{ii} = 0$, $\Lambda_i = \begin{cases} \frac{1}{2}, & i = 1, n \\ 1 & i = 2 \dots n - 1 \end{cases} \Rightarrow \text{estimate } |\lambda_i| \leq 1$

Gershgorin circles: heat example II

Let $n=11$, $h=0.1$:

$$\lambda_i = \cos\left(\frac{ih\pi}{1+2h}\right) \quad (i = 1 \dots n)$$



\Rightarrow the Gershgorin circle theorem is too pessimistic, we need a better theory ...

Permutation matrices

- ▶ Permutation matrices are matrices which have exactly one non-zero entry in each row and each column which has value 1.
- ▶ There is a one-to-one correspondence permutations π of the the numbers $1 \dots n$ and $n \times n$ permutation matrices $P = (p_{ij})$ such that

$$p_{ij} = \begin{cases} 1, & \pi(i) = j \\ 0, & \text{else} \end{cases}$$

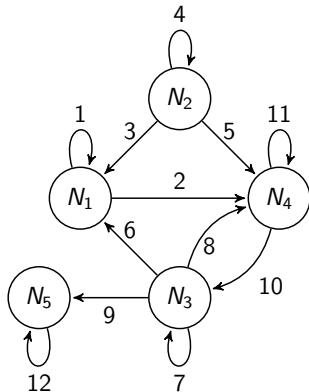
- ▶ Permutation matrices are orthogonal, and we have $P^{-1} = P^T$
- ▶ $A \rightarrow PA$ permutes the rows of A
- ▶ $A \rightarrow AP^T$ permutes the columns of A

Weighted directed graph representation of matrices

Define a directed graph from the nonzero entries of a matrix $A = (a_{ik})$:

- ▶ Nodes: $\mathcal{N} = \{N_i\}_{i=1\dots n}$
- ▶ Directed edges:
 $\mathcal{E} = \{\overrightarrow{N_k N_l} \mid a_{kl} \neq 0\}$
- ▶ Matrix entries \equiv weights of directed edges

$$A = \begin{pmatrix} 1. & 0. & 0. & 2. & 0. \\ 3. & 4. & 0. & 5. & 0. \\ 6. & 0. & 7. & 8. & 9. \\ 0. & 0. & 10. & 11. & 0. \\ 0. & 0. & 0. & 0. & 12. \end{pmatrix}$$



- ▶ 1:1 equivalence between matrices and weighted directed graphs
- ▶ Convenient e.g. for sparse matrices

Reducible and irreducible matrices

Definition A is *reducible* if there exists a permutation matrix P such that

$$PAP^T = \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix}$$

A is *irreducible* if it is not reducible.

Theorem (Varga, Th. 1.17): A is irreducible \Leftrightarrow the matrix graph is connected, i.e. for each *ordered* pair (N_i, N_j) there is a path consisting of directed edges, connecting them.

Equivalently, for each i, j there is a sequence of consecutive nonzero matrix entries $a_{ik_1}, a_{k_1k_2}, a_{k_2k_3}, \dots, a_{k_{r-1}k_r}, a_{k_rj}$.

□

Taussky theorem (Olga Taussky, 1948)

Theorem (Varga, Th. 1.18) Let A be irreducible. Assume that the eigenvalue λ is a boundary point of the union of all the disks

$$\lambda \in \partial \bigcup_{i=1 \dots n} \{\mu \in \mathbb{C} : |\mu - a_{ii}| \leq \Lambda_i\}$$

Then, all n Gershgorin circles pass through λ , i.e. for $i = 1 \dots n$,

$$|\lambda - a_{ii}| = \Lambda_i$$

Consequences for heat example from Taussky theorem

▶ $B = I - D^{-1}A$

▶ We had $b_{ii} = 0$, $\Lambda_i = \begin{cases} \frac{1}{2}, & i = 1, n \\ 1 & i = 2 \dots n-1 \end{cases} \Rightarrow \text{estimate } |\lambda_i| \leq 1$

▶ Assume $|\lambda_i| = 1$. Then λ_i lies on the boundary of the union of the Gershgorin circles. But then it must lie on the boundary of both circles with radius $\frac{1}{2}$ and 1 around 0.

▶ Contradiction $\Rightarrow |\lambda_i| < 1$, $\rho(B) < 1$!

Diagonally dominant matrices

Definition Let $A = (a_{ij})$ be an $n \times n$ matrix.

▶ A is *diagonally dominant* if

(i) for $i = 1 \dots n$, $|a_{ii}| \geq \sum_{\substack{j=1 \dots n \\ j \neq i}} |a_{ij}|$

▶ A is *strictly diagonally dominant* (sdd) if

(i) for $i = 1 \dots n$, $|a_{ii}| > \sum_{\substack{j=1 \dots n \\ j \neq i}} |a_{ij}|$

▶ A is *irreducibly diagonally dominant* (idd) if

(i) A is irreducible

(ii) A is diagonally dominant –

for $i = 1 \dots n$, $|a_{ii}| \geq \sum_{\substack{j=1 \dots n \\ j \neq i}} |a_{ij}|$

(iii) for at least one r , $1 \leq r \leq n$, $|a_{rr}| > \sum_{\substack{j=1 \dots n \\ j \neq r}} |a_{rj}|$

A very practical nonsingularity criterion

Theorem (Varga, Th. 1.21): Let A be strictly diagonally dominant or irreducibly diagonally dominant. Then A is nonsingular.

If in addition, $a_{ii} > 0$ is real for $i = 1 \dots n$, then all real parts of the eigenvalues of A are positive:

$$\operatorname{Re}\lambda_i > 0, \quad i = 1 \dots n$$

Corollary

Theorem: If A is complex hermitian or real symmetric, sdd or idd, with positive diagonal entries, it is positive definite.

Proof: All eigenvalues of A are real, and due to the nonsingularity criterion, they must be positive, so A is positive definite.



Perron-Frobenius Theorem (1912/1907)

Definition: A real n -vector \mathbf{x} is

- ▶ positive ($\mathbf{x} > 0$) if all entries of \mathbf{x} are positive
- ▶ nonnegative ($\mathbf{x} \geq 0$) if all entries of \mathbf{x} are nonnegative

Definition: A real $n \times n$ matrix A is

- ▶ positive ($A > 0$) if all entries of A are positive
- ▶ nonnegative ($A \geq 0$) if all entries of A are nonnegative

Theorem(Varga, Th. 2.7) Let $A \geq 0$ be an irreducible $n \times n$ matrix.
Then

- (i) A has a positive real eigenvalue equal to its spectral radius $\rho(A)$.
- (ii) To $\rho(A)$ there corresponds a positive eigenvector $\mathbf{x} > 0$.
- (iii) $\rho(A)$ increases when any entry of A increases.
- (iv) $\rho(A)$ is a simple eigenvalue of A .

Proof: See Varga. □

Perron-Frobenius for general nonnegative matrices

Each $n \times n$ matrix can be brought to the normal form

$$PAP^T = \begin{pmatrix} R_{11} & R_{12} & \dots & R_{1m} \\ 0 & R_{22} & \dots & R_{2m} \\ \vdots & & \ddots & \\ 0 & 0 & \dots & R_{mm} \end{pmatrix}$$

where for $j = 1 \dots m$, either R_{jj} irreducible or $R_{jj} = (0)$.

Theorem(Varga, Th. 2.20) Let $A \geq 0$ be an $n \times n$ matrix. Then

- (i) A has a nonnegative eigenvalue equal to its spectral radius $\rho(A)$. This eigenvalue is positive unless A is reducible and its normal form is strictly upper triangular
- (ii) To $\rho(A)$ there corresponds a nonzero eigenvector $\mathbf{x} \geq 0$.
- (iii) $\rho(A)$ does not decrease when any entry of A increases.

Proof: See Varga; $\sigma(A) = \bigcup_{j=1}^m \sigma(R_{jj})$, apply irreducible Perron-Frobenius to R_{jj} . □

Theorem on Jacobi matrix

Theorem: Let A be sdd or idd, and D its diagonal. Then

$$\rho(|I - D^{-1}A|) < 1$$

Proof: Let $B = (b_{ij}) = I - D^{-1}A$. Then

$$b_{ij} = \begin{cases} 0, & i = j \\ -\frac{a_{ij}}{a_{ii}}, & i \neq j \end{cases}$$

If A is sdd, then for $i = 1 \dots n$,

$$\sum_{j=1 \dots n} |b_{ij}| = \sum_{\substack{j=1 \dots n \\ j \neq i}} \left| \frac{a_{ij}}{a_{ii}} \right| = \frac{\Lambda_i}{|a_{ii}|} < 1$$

Therefore, $\rho(|B|) < 1$.

Jacobi method convergence

Corollary: Let A be sdd or idd, and D its diagonal. Assume that $a_{ii} > 0$ and $a_{ij} \leq 0$ for $i \neq j$. Then $\rho(I - D^{-1}A) < 1$, i.e. the Jacobi method converges.

Proof In this case, $|B| = B$ □.

- ▶ Here, we made assumptions on the sign pattern and the diagonal dominance of the matrix. No additional information on the nonzero pattern or the symmetry has been used.
- ▶ Does this generalize to other iterative methods ?

Regular splittings

- ▶ $A = M - N$ is a regular splitting if
 - ▶ M is nonsingular
 - ▶ M^{-1} , N are nonnegative, i.e. have nonnegative entries
- ▶ Regard the iteration $u_{k+1} = M^{-1}Nu_k + M^{-1}b$.
- ▶ $B = I - M^{-1}A = M^{-1}N$ is a nonnegative matrix.

Convergence theorem for regular splitting

Theorem: Assume A is nonsingular, $A^{-1} \geq 0$, and $A = M - N$ is a regular splitting. Then $\rho(M^{-1}N) < 1$.

Proof: Let $B = M^{-1}N$. Then $A = M(I - B)$, therefore $I - B$ is nonsingular.

In addition

$$A^{-1}N = (M(I - M^{-1}N))^{-1}N = (I - M^{-1}N)^{-1}M^{-1}N = (I - B)^{-1}B$$

By Perron-Frobenius (for general matrices), $\rho(B)$ is an eigenvalue with a nonnegative eigenvector \mathbf{x} . Thus,

$$0 \leq A^{-1}N\mathbf{x} = \frac{\rho(B)}{1 - \rho(B)}\mathbf{x}$$

Therefore $0 \leq \rho(B) \leq 1$.

Assume that $\rho(B) = 1$. Then there exists $\mathbf{x} \neq \mathbf{0}$ such that $B\mathbf{x} = \mathbf{x}$.

Consequently, $(I - B)\mathbf{x} = \mathbf{0}$, contradicting the nonsingularity of $I - B$.

Therefore, $\rho(B) < 1$. □

Convergence rate comparison

Corollary: $\rho(M^{-1}N) = \frac{\tau}{1+\tau}$ where $\tau = \rho(A^{-1}N)$.

Proof: Rearrange $\tau = \frac{\rho(B)}{1-\rho(B)}$ \square

Corollary: Let $A^{-1} \geq 0$, $A = M_1 - N_1$ and $A = M_2 - N_2$ be regular splittings.

If $N_2 \geq N_1$, then $1 > \rho(M_2^{-1}N_2) \geq \rho(M_1^{-1}N_1)$.

Proof: $\tau_2 = \rho(A^{-1}N_2) \geq \rho(A^{-1}N_1) = \tau_1$

But $\frac{\tau}{1+\tau}$ is strictly increasing. \square

Convergence rate comparison II

- ▶ Let $A^{-1} \geq 0$, $A = D - E - F$, $D > 0$ diagonal, $E, F \geq 0$ upper resp. lower triangular parts.
- ▶ Jacobi: $M_J = D$, $N_J = E + F$. $M_J^{-1} > 0 \Rightarrow$ regular splitting
- ▶ Gauss-Seidel: $M_{GS} = D - E$, $N_{GS} = F \geq 0$. Show $M_{GS}^{-1} \geq 0$:

$$M_{GS} = \begin{pmatrix} d_{11} & -e_{12} & -e_{13} & \dots & -e_{1n} \\ & d_{22} & -e_{23} & \dots & -e_{2n} \\ & & \ddots & \ddots & \vdots \\ & & & d_{n-1,n-1} & -e_{n-1,n} \\ & & & \dots & d_{nn} \end{pmatrix}$$

Elimination steps for $M_{GS}v = r$:

$$v_n = \frac{r_n}{d_{nn}}, \quad v_{n-1} = \frac{r_n + e_{n-1,n}v_n}{d_{n-1,n-1}} \dots$$

All coefficients are nonnegative $\Rightarrow M_{GS} - N_{GS}$: regular splitting

- ▶ $N_{GS} \leq N_J \Rightarrow \rho(M_{GS}^{-1}N_{GS}) \leq \rho(M_J^{-1}N_J)$

M-Matrix definition

Definition Let A be an $n \times n$ real matrix. A is called M-Matrix if

- (i) $a_{ij} \leq 0$ for $i \neq j$
- (ii) A is nonsingular
- (iii) $A^{-1} \geq 0$

Corollary: If A is an M-Matrix, then $A^{-1} > 0 \Leftrightarrow A$ is irreducible.

Proof: See Varga. □

M-Matrix main diagonal

Theorem: If A is an M -matrix, then its diagonal $D_A > 0$ is positive.

Proof: Let $C = A^{-1} \geq 0$. Then $AC = I$ and $(AC)_{ii} = 1$.

$$\sum_{k=1}^n a_{ik} c_{ki} = 1$$

$$a_{ij} c_{ij} = 1 - \sum_{k=1, k \neq i}^n a_{ik} c_{ki} \geq 1$$

The last inequality is due to $c_{ki} \geq 0$ and $a_{ik} < 0$ for $k \neq i$. As $a_{ij} c_{ij} \geq 1$, neither factor can be 0. So $c_{ij} > 0$ and $a_{ij} > 0$.

Theorem: (Saad, Th. 1.31) Assume

(i) $a_{ij} \leq 0$ for $i \neq j$

(ii) $a_{ii} > 0$

Then A is an M -Matrix if and only if $\rho(I - D^{-1}A) < 1$.

Proof: See Saad.



Main practical M-Matrix criterion

Corollary: Let A be sdd or idd. Assume that $a_{ii} > 0$ and $a_{ij} \leq 0$ for $i \neq j$. Then A is an M-Matrix.

Proof: We know that A is nonsingular, but we have to show $A^{-1} \geq 0$.

- ▶ Let $B = I - D^{-1}A$. Then $\rho(B) < 1$, therefore $I - B$ is nonsingular.
- ▶ We have for $k > 0$:

$$\begin{aligned}I - B^{k+1} &= (I - B)(I + B + B^2 + \dots + B^k) \\(I - B)^{-1}(I - B^{k+1}) &= (I + B + B^2 + \dots + B^k)\end{aligned}$$

The left hand side for $k \rightarrow \infty$ converges to $(I - B)^{-1}$, therefore

$$(I - B)^{-1} = \sum_{k=0}^{\infty} B^k$$

As $B \geq 0$, we have $(I - B)^{-1} = A^{-1}D \geq 0$. As $D > 0$ we must have $A^{-1} \geq 0$. □

M-Matrix comparison criterion

Theorem(Saad, Th. 1.33): Let A, B $n \times n$ matrices such that

(i) $A \leq B$

(ii) $b_{ij} \leq 0$ for $i \neq j$.

Then, if A is an M-Matrix, so is B .

Proof: From M-property of A and $A \leq B$ we have $0 < D_A \leq D_B$. We have $D_B - B \geq 0$ and

$$\begin{aligned}D_A - A &\geq D_B - B \\I - D_A^{-1}A &\geq D_A^{-1}(D_B - B) \\&\geq D_B^{-1}(D_B - B) \\&\geq I - D_B^{-1}B =: G \geq 0\end{aligned}$$

Perron-Frobenius $\Rightarrow \rho(G) = \rho(I - D_B^{-1}B) \leq \rho(I - D_A^{-1}A) < 1$
 $\Rightarrow I - G$ is nonsingular. From the proof of the M-matrix criterion,
 $D_B^{-1}B = (I - G)^{-1} = \sum_{k=0}^{\infty} G^k \geq 0$. As $D_B > 0$, we get $B \geq 0$.

□

Corollary $A \leq M_{GS} \Rightarrow M_{GS}$ is an M-Matrix.

Incomplete LU factorizations (ILU)

Idea (Varga, Buleev, 1960):

- ▶ fix a predefined zero pattern
- ▶ apply the standard LU factorization method, but calculate only those elements, which do not correspond to the given zero pattern
- ▶ Result: incomplete LU factors L , U , remainder R :

$$A = LU - R$$

- ▶ Problem: with complete LU factorization procedure, for any nonsingular matrix, the method is stable, i.e. zero pivots never occur. Is this true for the incomplete LU Factorization as well ?

M-Property propagation in Gaussian Elimination

Theorem:(Ky Fan; Saad Th 1.10) Let A be an M-matrix. Then the matrix A_1 obtained from the first step of Gaussian elimination is an M-matrix.

Proof: One has $a_{ij}^1 = a_{ij} - \frac{a_{i1}a_{1j}}{a_{11}}$,
 $a_{ij}, a_{i1}, a_{1j} \leq 0, a_{11} > 0$
 $\Rightarrow a_{ij}^1 \leq 0$ for $i \neq j$

$$A = L_1 A_1 \text{ with } L_1 = \begin{pmatrix} 1 & 0 & \dots & 0 \\ \frac{-a_{12}}{a_{11}} & 1 & \dots & 0 \\ \vdots & & \ddots & 0 \\ \frac{-a_{1n}}{a_{11}} & 0 & \dots & 1 \end{pmatrix} \text{ nonsingular, nonnegative}$$

$\Rightarrow A_1$ nonsingular

Let $e_1 \dots e_n$ be the unit vectors. Then $A_1^{-1}e_1 = \frac{1}{a_{11}}e_1 \geq 0$. For $j > 1$,
 $A_1^{-1}e_j = A^{-1}L^{-1}e_j = A^{-1}e_j \geq 0$.
 $\Rightarrow A_1^{-1} \geq 0$



Stability of ILU

Theorem (Saad, Th. 10.2): If A is an M-Matrix, then the algorithm to compute the incomplete LU factorization with a given nonzero pattern

$$A = LU - R$$

is stable. Moreover, $A = LU - R$ is a regular splitting.

Stability of ILU decomposition II

Proof

Let $\tilde{A}_1 = A_1 + R_1 = L_1 A + R_1$ where R_1 is a nonnegative matrix which occurs from dropping some off diagonal entries from A_1 . Thus, $\tilde{A}_1 \geq A_1$ and \tilde{A}_1 is an M-matrix. We can repeat this recursively

$$\begin{aligned}\tilde{A}_k &= A_k + R_k = L_k A_{k-1} + R_k \\ &= L_k L_{k-1} A_{k-2} + L_k R_{k-1} + R_k \\ &= L_k L_{k-1} \cdot \dots \cdot L_1 A + L_k L_{k-1} \cdot \dots \cdot L_2 R_1 + \dots + R_k\end{aligned}$$

Let $L = (L_{n-1} \cdot \dots \cdot L_1)^{-1}$, $U = \tilde{A}_{n-1}$. Then $U = L^{-1}A + S$ with

$$S = L_{n-1} L_{n-2} \cdot \dots \cdot L_2 R_1 + \dots + R_{n-1} = L_{n-1} L_{n-2} \cdot \dots \cdot L_2 (R_1 + R_2 + \dots + R_{n-1})$$

Let $R = R_1 + R_2 + \dots + R_{n-1}$, then $A = LU - R$ where $U^{-1}L^{-1}$, R are nonnegative.



ILU(0)

- ▶ Special case of ILU: ignore any fill-in.
- ▶ Representation:

$$M = (\tilde{D} - E)\tilde{D}^{-1}(\tilde{D} - F)$$

- ▶ \tilde{D} is a diagonal matrix (which can be stored in one vector) which is calculated by the incomplete factorization algorithm.
- ▶ Setup:

```
for i=1:n
    d[i]=a[i,i]
end

for i=1:n
    d[i]=1.0/d[i]
    for j=i+1:n
        d[j]=d[j]-a[i,j]*d[i]*a[j,i]
    end
end
```

ILU(0)

Solve $Mu = v$

```
for i=1:n
    x=0.0
    for j=1:i-1
        x=x+a[i,j]*u[j]
        u[i]=d[i]*(v[i]-x)
    end
end
for i=n:-1:1
    x=0.0
    for j=i+1:n
        x=x+a[i,j]*u[j]
        u[i]=u[i]-d[i]*x
    end
end
```

ILU(0)

- ▶ Generally better convergence properties than Jacobi, Gauss-Seidel
- ▶ One can develop block variants
- ▶ Alternatives:
 - ▶ ILUM: (“modified”): add ignored off-diagonal entries to \tilde{D}
 - ▶ ILUT: zero pattern calculated dynamically based on drop tolerance
- ▶ Dependence on ordering
- ▶ Can be parallelized using graph coloring
- ▶ Not much theory: experiment for particular systems
- ▶ I recommend it as the default initial guess for a sensible preconditioner
- ▶ Incomplete Cholesky: symmetric variant of ILU

Intermediate Summary

- ▶ Given some matrix, we now have some nice recipes to establish nonsingularity and iterative method convergence:
- ▶ **Check if the matrix is irreducible.**
This is mostly the case for elliptic and parabolic PDEs.
- ▶ **Check if the matrix is strictly or irreducibly diagonally dominant.**
If yes, it is in addition nonsingular.
- ▶ **Check if main diagonal entries are positive and off-diagonal entries are nonpositive.**
If yes, in addition, the matrix is an M-Matrix, its inverse is nonnegative, and elementary iterative methods converge.
- ▶ These criteria do not depend on the symmetry of the matrix!

