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Lecture 8

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Recap: iterative methods

Simple iteration with preconditioning

Idea: $A\hat{u} = b \Rightarrow$

$$\hat{u} = \hat{u} - M^{-1}(A\hat{u} - b)$$

$\Rightarrow$ iterative scheme

$$u_{k+1} = u_k - M^{-1}(Au_k - b) \quad (k = 0, 1 \dots)$$

1. Choose initial value u_0, tolerance ε, set $k = 0$
2. Calculate *residuum* $r_k = Au_k - b$
3. Test convergence: if $||r_k|| < \varepsilon$ set $u = u_k$, finish
4. Calculate *update*: solve $Mv_k = r_k$
5. Update solution: $u_{k+1} = u_k - v_k$, set $k = i + 1$, repeat with step 2.

The Jacobi method

- Let $A = D - E - F$, where D: main diagonal, E: negative lower triangular part F: negative upper triangular part
- Preconditioner: $M = D$, where D is the main diagonal of $A \Rightarrow$

$$u_{k+1,i} = u_{k,i} - \frac{1}{a_{ii}} \left(\sum_{j=1\ldots n} a_{ij} u_{k,j} - b_i \right) \quad (i = 1 \ldots n)$$

- Equivalent to the succesive (row by row) solution of

$$a_{ii} u_{k+1,i} + \sum_{j=1\ldots n, j\neq i} a_{ij} u_{k,j} = b_i \quad (i = 1 \ldots n)$$

- Already calculated results not taken into account
- Alternative formulation with $A = M - N$:

$$\begin{aligned} u_{k+1} &= D^{-1}(E + F)u_k + D^{-1}b \\ &= M^{-1}Nu_k + M^{-1}b \end{aligned}$$

- Variable ordering does not matter

Convergence

- Let $\hat{u}$ be the solution of $Au = b$.
- Let $e_k = u_j - \hat{u}$ be the error of the k-th iteration step

$$\begin{aligned} u_{k+1} &= u_k - M^{-1}(Au_k - b) \\ &= (I - M^{-1}A)u_k + M^{-1}b \\ u_{k+1} - \hat{u} &= u_k - \hat{u} - M^{-1}(Au_k - A\hat{u}) \\ &= (I - M^{-1}A)(u_k - \hat{u}) \\ &= (I - M^{-1}A)^k(u_0 - \hat{u}) \end{aligned}$$

resulting in

$$e_{k+1} = (I - M^{-1}A)^k e_0$$

- So when does $(I - M^{-1}A)^k$ converge to zero for $k \to \infty$?

Back to iterative methods

Sufficient condition for convergence: $\rho(I - M^{-1}A) < 1$.

Richardson for 1D heat conduction

- Regard the $n \times n$ 1D heat conduction matrix with $h = \frac{1}{n-1}$ and $\alpha = \frac{1}{h}$ (easier to analyze).

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

- Eigenvalues (tri-diagonal Toeplitz matrix):

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

Source: A. Böttcher, S. Grudsky: Spectral Properties of Banded Toeplitz Matrices. SIAM,2005

- Express them in h: $n + 1 = \frac{1}{h} + 2 = \frac{1+2h}{h} \Rightarrow$

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

Richardson for 1D heat conduction: Jacobi

- The Jacobi preconditioner just multiplies by $\frac{h}{2}$, therefore for $M^{-1}A$:

$$\lambda_{max} \approx 2 - \frac{\pi^2 h^2}{2(1+2h)^2}$$
$$\lambda_{min} \approx \frac{\pi^2 h^2}{2(1+2h)^2}$$

- Optimal parameter: $\alpha = \frac{2}{\lambda_{max}+\lambda_{min}} \approx 1 \; (h \to 0)$
- Good news: this is independent of h resp. n
- No need for spectral estimate in order to work with optimal parameter
- Is this true beyond this special case ?

Richardson for 1D heat conduction: Convergence factor

- Condition number + spectral radius

$$\kappa(M^{-1}A) = \kappa(A) = \frac{4(1+2h)^2}{\pi^2 h^2} - 1$$

$$\rho(I - M^{-1}A) = \frac{\kappa - 1}{\kappa + 1} = 1 - \frac{\pi^2 h^2}{2(1+2h)^2}$$

- Bad news: $\rho \to 1 \quad (h \to 0)$
- Typical situation with second order PDEs:

$$\kappa(A) = O(h^{-2}) \quad (h \to 0)$$

$$\rho(I - D^{-1}A) = 1 - O(h^2) \quad (h \to 0)$$

Iterative solver complexity I

- Solve linear system iteratively until $||e_k|| = ||(I - M^{-1}A)^k e_0|| \leq \epsilon$

$$
\begin{aligned}
\rho^k e_0 &\leq \epsilon \\
k \ln \rho &< \ln \epsilon - \ln e_0 \\
k \geq k_\rho &= \left\lceil \frac{\ln e_0 - \ln \epsilon}{\ln \rho} \right\rceil
\end{aligned}
$$

- Assume $\rho < \rho_0 < 1$ independent of h resp. N, A sparse and solution of $Mv = r$ has complexity $O(N)$.
  $\Rightarrow$ Number of iteration steps k_ρ independent of N
  $\Rightarrow$ Overall complexity $O(N)$.

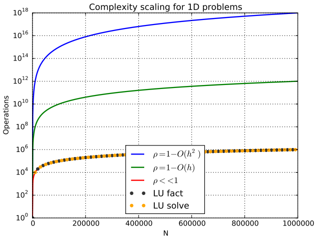
Iterative solver complexity II

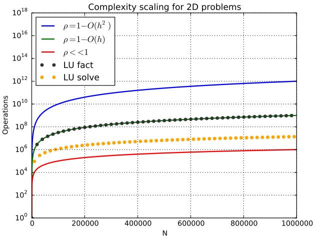
- Assume $\rho = 1 - h^\delta \Rightarrow \ln\rho \approx -h^\delta$
- $k = O(h^{-\delta})$
- d: space dimension, then $h \approx N^{-\frac{1}{d}} \Rightarrow k = O(N^{\frac{\delta}{d}})$
- Assume $O(N)$ complexity of one iteration step
  $\Rightarrow$ Overall complexity $O(N^{\frac{d+\delta}{d}})$
- Jacobi: $\delta = 2$, something better with at least $\delta = 1$?

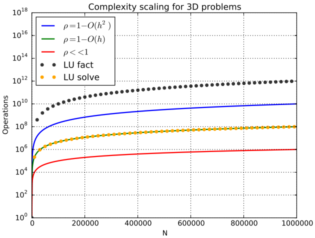
dim	$\rho = 1 - O(h^2)$	$\rho = 1 - O(h)$	LU fact.	LU solve
1	$O(N^3)$	$O(N^2)$	$O(N)$	$O(N)$
2	$O(N^2)$	$O(N^{\frac{3}{2}})$	$O(N^{\frac{3}{2}})$	$O(N\log N)$
3	$O(N^{\frac{5}{3}})$	$O(N^{\frac{4}{3}})$	$O(N^2)$	$O(N^{\frac{4}{3}})$

- In 1D, iteration makes not much sense
- In 2D, we can hope for parity
- In 3D, beat sparse matrix solvers with $\rho = 1 - O(h)$?

Solver complexity: scaling with problem size

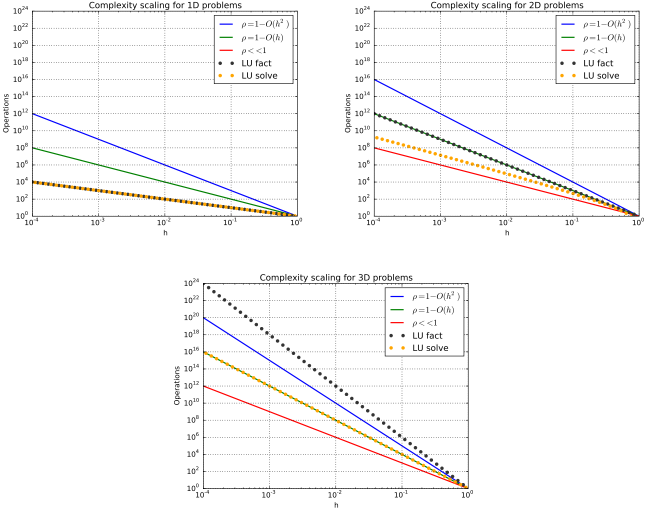






Scaling with problem size.

Solver complexity: scaling with accuracy



- Accuracy of numerial solutions is proportional to some power of h.
- Amount of operations for to reach a given accuracy.

What could be done ?

- Find a better preconditioner with $\kappa(M^{-1}A) = O(h^{-1})$ or independent of h
- Find a better iterative scheme:
  Assume e.g. $\rho = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$. Let $\kappa = X^2 - 1$ where $X = \frac{2(1+2h)}{\pi h} = O(h^{-1})$.

$$
\begin{aligned}
\rho &= 1 + \frac{\sqrt{X^2-1}-1}{\sqrt{X^2-1}+1} - 1 \\
&= 1 + \frac{\sqrt{X^2-1}-1-\sqrt{X^2-1}-1}{\sqrt{X^2-1}+1} \\
&= 1 - \frac{1}{\sqrt{X^2-1}+1} \\
&= 1 - \frac{1}{X\left(\sqrt{1-\frac{1}{X^2}}+\frac{1}{X}\right)} \\
&= 1 - O(h)
\end{aligned}
$$

- Here, we would have $\delta = 1$. Together with a good preconditioner ...

Eigenvalue analysis for more general matrices

- For 1D heat conduction we used a very special regular structure of the matrix which allowed exact eigenvalue calculations
- Generalizations to tensor product is possible
- Generalization to varying coefficients, unstructured grids ...
  $\Rightarrow$ what can be done for general matrices ?

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

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

If λ is an eigenvalue of A then there exists r, $1 \leq r \leq n$ such that

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

Proof Assume λ is eigenvalue, $\mathbf{x}$ a corresponding eigenvector, normalized such that $\max_{i=1\dots n} |x_i| = |x_r| = 1$. From $A\mathbf{x} = \lambda \mathbf{x}$ it follows that

$$(\lambda - a_{ii})x_i = \sum_{\substack{j=1\dots n \\ j \neq i}} a_{ij} x_j$$

$$|\lambda - a_{rr}| = |\sum_{\substack{j=1\dots n \\ j \neq r}} a_{rj} x_j| \leq \sum_{\substack{j=1\dots n \\ j \neq r}} |a_{rj}||x_j| \leq \sum_{\substack{j=1\dots n \\ j \neq r}} |a_{rj}| = \Lambda_r$$

$\square$

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:

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

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

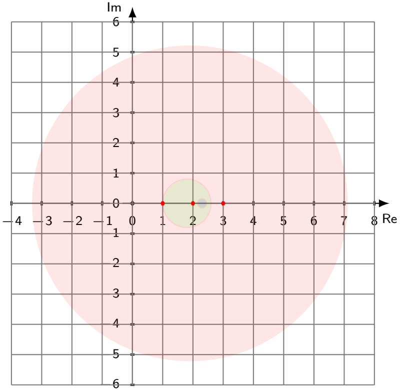
Proof

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

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

Gershgorin circles: example

$$A = \begin{pmatrix} 1.9 & 1.8 & 3.4 \\ 0.4 & 1.8 & 0.4 \\ 0.05 & 0.1 & 2.3 \end{pmatrix}, \lambda_1 = 1, \lambda_2 = 2, \lambda_3 = 3, \Lambda_1 = 5.2, \Lambda_2 = 0.8, \lambda_3 = 0.15$$



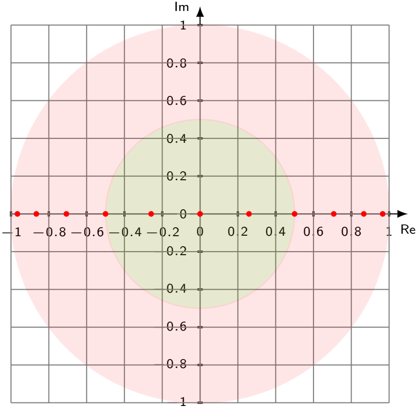
Gershgorin circles: heat example I

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

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

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

Gershgorin circles: heat example II



n=11, h=0.1

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

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.

Directed matrix graph:

- Nodes: $\mathcal{N} = \{N_i\}_{i=1\dots n}$
- Directed edges: $\mathcal{E} = \{\overrightarrow{N_k N_l} | a_{kl} \neq 0\}$

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 nonzero matrix entries $a_{ik_1}, a_{k_1 k_2}, \dots, a_{k_r j}$.

□

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 $i = 1 \dots n$,

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

Taussky theorem proof

Proof Assume λ is eigenvalue, $\mathbf{x}$ a corresponding eigenvector, normalized such that $\max_{i=1\dots n}|x_i| = |x_r| = 1$. From $A\mathbf{x} = \lambda\mathbf{x}$ it follows that

$$|\lambda - a_{rr}| \le \sum_{\substack{j=1\dots n\\ j\neq r}} |a_{rj}|\cdot|x_j| \le \sum_{\substack{j=1\dots n\\ j\neq r}} |a_{rj}| = \Lambda_r \qquad (*)$$

Boundary point $\Rightarrow |\lambda - a_{rr}| = \Lambda_r$

$\Rightarrow$ For all $l \neq r$ with $a_{r,p} \neq 0$, $|x_p| = 1$.

Due to irreducibility there is at least one such p. For this p, equation $(*)$ is valid (with p in place of r) $\Rightarrow |\lambda - a_{pp}| = \Lambda_p$

Due to irreducibility, this is true for all $p = 1\dots n$. $\square$

Consequences for heat example from Taussky

$B = I - D^{-1}A$

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

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

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

A very practical nonsingularity criterion, proof

Proof:

- Assume A sdd. Then the union of the Gershgorin disks does not contain 0 and $\lambda = 0$ cannot be an eigenvalue.

  As for the real parts, the union of the disks is

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

  and $\mathrm{Re}\mu$ must be larger than zero if μ should be contained.

- Assume A idd. Then, if 0 is an eigenvalue, it sits on the boundary of one of the Gershgorin disks. By the Taussky theorem, we have $|a_{ii}| = \Lambda_i$ for all $i = 1 \dots n$. This is a contradiction as by definition there is at least one i such that $|a_{ii}| > \Lambda_i$

  Assume $a_{ii} > 0$, real. All real parts of the eigenvalues must be ≥ 0. Therefore, if a real part is 0, it lies on the boundary of one disk. So by Taussky it must be contained at the same time in the boundary of all the disks and the imaginary axis. This contradicts the fact that there is at least one disk which does not touch the imaginary axis.

$\square$

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.

$\square$

Heat conduction matrix

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

- A is idd $\Rightarrow$ A is nonsingular
- $\mathrm{diag} A$ is positive real $\Rightarrow$ eigenvalues of A have positive real parts
- A is real, symmetric $\Rightarrow$ 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. $\square$

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 $i = 1 \dots n$,

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

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

Theorem on Jacobi matrix II

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

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

$$\sum_{j=1\dots n} |b_{rj}| = \frac{\Lambda_r}{|a_{rr}|} < 1 \text{ for at least one } r$$

Therefore, $\rho(|B|) <= 1$. Assume $\rho(|B|) = 1$. By Perron-Frobenius, 1 is an eigenvalue. As it is in the union of the Gershgorin disks, for some i,

$$|\lambda| = 1 \leq \frac{\Lambda_i}{|a_{ii}|} \leq 1$$

and it must lie on the boundary of this union. By Taussky then one has for all i

$$|\lambda| = 1 \leq \frac{\Lambda_i}{|a_{ii}|} = 1$$

which contradicts the idd condition. $\square$

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, $|B| = B$ $\square$.

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 $u_{k+1} = M^{-1}Nu_k + M^{-1}b$.
- We have $I - M^{-1}A = M^{-1}N$.

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 $G = M^{-1}N$. Then $A = M(I - G)$, therefore $I - G$ is nonsingular.

In addition

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

By Perron-Frobenius, $\rho(G)$ is an eigvenalue with a nonnegative eigenvector $\mathbf{x}$. Thus,

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

Therefore $0 \leq \rho(G) \leq 1$.
As $I - G$ is nonsingular, $\rho(G) < 1$. $\square$

Convergence rate comparison

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

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

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

Proof: $\tau_2 = \rho(A^{-1}N_2) \geq \rho(A^{-1}N_1) = \tau_1$, $\frac{\tau}{1+\tau}$ is strictly increasing.

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. $\square$

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:

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

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

The left hand side for $k \to \infty$ 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 $A^{-1} \geq 0$. $\square$

Application

Let A be an M-Matrix. Assume $A = D - E - F$.

- Jacobi method: $M = D$ is nonsingular, $M^{-1} \geq 0$. $N = E + F$ nonnegative $\Rightarrow$ convergence
- Gauss-Seidel: $M = D - E$ is an M-Matrix as $A \leq M$ and M has non-positive off-digonal entries. $N = F \geq 0$. $\Rightarrow$ convergence
- Comparison: $N_J \geq N_{GS} \Rightarrow$ Gauss-Seidel converges faster.
- More general: Block Jacobi, Block Gauss Seidel etc.

Intermediate Summary

- Given some matrix, we now have some nice recipies 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.

Example: 1D finite volume matrix:

$$Au = \begin{pmatrix} \alpha + \frac{1}{h} & -\frac{1}{h} & & & & & \\ -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & & & \\ & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & & \\ & \ddots & \ddots & \ddots & \ddots & & \\ & & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & \\ & & & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & \\ & & & & -\frac{1}{h} & \frac{1}{h} + \alpha \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \\ u_N \end{pmatrix} = f = \begin{pmatrix} \alpha v_1 \\ hf_2 \\ hf_3 \\ \vdots \\ hf_{N-2} \\ hf_{N-1} \\ \alpha v_n \end{pmatrix}$$

- idd
- positive main diagonal entries, nonpositive off-diagonal entries

$\Rightarrow$ A is nonsingular, has the M-property, and we can e.g. apply the Jacobi and Gauss-Seidel iterative method to solve it.

$\Rightarrow$ for $f \geq 0$ and $v \geq 0$ it follows that $u \geq 0$.
$\equiv$ heating and positive environment temperatures cannot lead to negative temperatures in the interior.