Singularity of the discrete Laplacian operator

Andrea Alessandro Ruggiu   Jan Nordström

LINKÖPING UNIVERSITY

Motivation

In the SBP–SAT framework, for unsteady initial boundary value problems we can usually state

continuous well–posedness $\Rightarrow$ stable discretization

Such properties are related to the sign of the eigenvalues of spatial operators being nonpositive (or nonnegative), both in the continuous and discrete settings.

$$u_t + Lu = f, \quad x \in \Omega, \quad t > 0 \quad \rightarrow \quad \mathbf{v}_t + L_D\mathbf{v} = \mathbf{f}, \quad t > 0.$$

$$\text{eig}\,(L) \geq 0 \quad \Rightarrow \quad \text{eig}\,(L_D) \geq 0.$$

The continuous problem

Consider the one–dimensional Poisson equation with two boundary conditions

$$
\begin{aligned}
-u_{xx} &= F(x), \quad && 0 < x < 1, \\
L_0 u(0) := \left(a_0 + b_0 \tfrac{\partial}{\partial x}\right) u(0) &= g_0, && a_0, b_0 \in \mathbb{R}, \\
L_1 u(1) := \left(a_1 + b_1 \tfrac{\partial}{\partial x}\right) u(1) &= g_1, && a_1, b_1 \in \mathbb{R}.
\end{aligned}
$$

The solution to is not unique if, and only if,

$$a_0 (a_1 + b_1) - a_1 b_0 = 0. \tag{1}$$

Proof

The solution consists of two parts

$$u(x) = \underbrace{c_0 + c_1 x}_{\text{homogeneous}} + \underbrace{u_p(x)}_{\text{particular}}, \quad c_0, c_1 \in \mathbb{R}, \qquad (2)$$

where $u_p(x) = u_p(F(x))$ does not depend on the boundary conditions.
By applying the boundary conditions to (2) leads to

$$E \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} = \begin{bmatrix} a_0 & b_0 \\ a_1 & a_1 + b_1 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} = \begin{bmatrix} g_0 - L_0 u_p(0) \\ g_1 - L_1 u_p(1) \end{bmatrix}.$$

The condition $det(E) = 0$ yields (1).

Recalling some theory

Let $T \in \mathbb{R}^{m \times n}$. Then we define

Definition (Rank and Nullspace of a matrix)

The number of linearly independent rows (or columns) of T is said to be the rank of T and it is denoted $rk\,(T)$. The null space of T is the set

$$nul\,(T) = \{\mathbf{w} \in \mathbb{R}^n : T\mathbf{w} = \mathbf{0}\}\,.$$

Remark (Subadditivity of the rank)

The rank is *subadditive*: if A and B are matrices of the same dimensions, then

$$rk\,(A+B) \leq rk\,(A) + rk\,(B)\,.$$

Theorem (Rank–nullity theorem)

The rank and dimension of the null space of T sums to the number of its columns, i.e.

$$rk\,(T) + dim\,(nul\,(T)) = n.$$

Therefore a square matrix is non–singular if, and only if, $dim\,(nul\,(T)) = 0$.

Recalling Summation–By–Parts operators

Definition

$D = P^{-1}Q$ is a first–derivative SBP operator if $Q + Q^T = B = diag\,(-1, 0, \ldots, 0, 1)$ and P is a symmetric positive definite matrix.

Definition

$D_2 = P^{-1}\left(-S^T M + B\right) S$ is a second–derivative SBP operator if M is positive semidefinite and S approximates the first derivative operator at the boundaries.

The discrete problem

Simultaneous–Approximation–Terms (SAT) enforces the boundary conditions weakly.

The SBP–SAT approximation of the Poisson problem can be formally written as

$$-D_2\mathbf{v} = \mathbf{F} + SAT, \quad D_2 \in \mathbb{R}^{(N+1)\times(N+1)} \tag{3}$$

where SAT collects the penalty terms of the discretization.

Consider the following SAT term

$$\begin{aligned} SAT = & -\alpha_0 P^{-1} E_0 \left[\left(a_0 I + b_0 S \right) \mathbf{v} - \mathbf{g}_0 \right] \\ & + \alpha_N P^{-1} E_N \left[\left(a_1 I + b_1 S \right) \mathbf{v} - \mathbf{g}_1 \right], \end{aligned}$$

where we have used $\alpha_0, \alpha_N \in \mathbb{R}$, $E_0 = diag\,(1, 0, \ldots, 0)$, $E_N = diag\,(0, \ldots, 0, 1) \in \mathbb{R}^{(N+1)\times(N+1)}$.

The discrete Poisson problem is $A\mathbf{v} = \mathbf{G}$, where

$$A = D_2 - \alpha_0 P^{-1} E_0 \left(a_0 I + b_0 S \right) + \alpha_N P^{-1} E_N \left(a_1 I + b_1 S \right).$$

Note: $\mathbf{G}$ is independent of $\mathbf{v}$.

A reasonable assumption

We require that

$$\begin{aligned} \mathbf{1} &= [1,\ldots,1]^T &\Rightarrow \quad D\mathbf{1} &= \mathbf{0}, \quad & D_2\mathbf{1} &= \mathbf{0}, \\ \mathbf{x} &= h\,[0,\ldots,N]^T &\Rightarrow \quad D\mathbf{x} &= \mathbf{1}, \quad & D_2\mathbf{x} &= \mathbf{0}. \end{aligned} \tag{4}$$

Ill–posedness implies singularity

Theorem : ill–posedness $\Rightarrow$ A singular

Proof: Let $\mathbf{y} = \beta\mathbf{1} + \gamma\mathbf{x}$, with $(\beta, \gamma) \in \mathbb{R}^2 \setminus \{(0,0)\}$.
Since $D_2\mathbf{y} = \mathbf{0}$ and P is positive definite, we can write

$$A\mathbf{y} = \mathbf{0} \quad \Rightarrow \quad \begin{aligned} (a_0 I + b_0 S)\,\mathbf{y} &= 0, \\ (a_1 I + b_1 S)\,\mathbf{y} &= 0. \end{aligned}$$

Substituting $\mathbf{y}$ and using (4), we get

$$E\begin{bmatrix}\beta\\ \gamma\end{bmatrix} = \begin{bmatrix} a_0 & b_0 \\ a_1 & a_1 + b_1 \end{bmatrix}\begin{bmatrix}\beta\\ \gamma\end{bmatrix} = \begin{bmatrix}0\\ 0\end{bmatrix} \quad \overset{det(E)=0}{\Rightarrow} \quad (1).$$

Numerical check

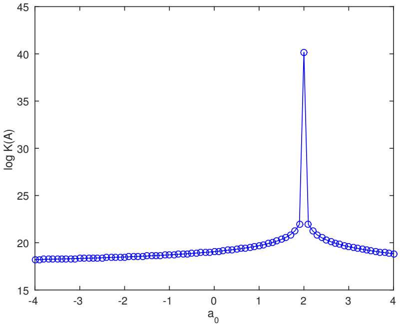

Figure: $b_0 = 4$, $a_1 = 1$, $b_1 = 1$. With this choice (1) is satisfied for $a_0 = 2$.

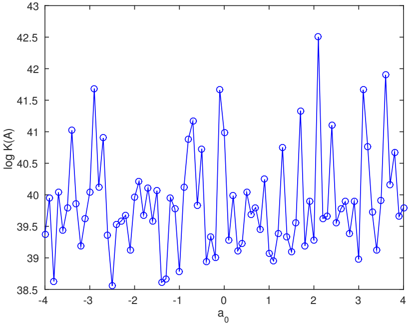

Figure: $b_0 = 0$, $a_1 = 1$, $b_1 = -1$. With this choice (1) is satisfied for any $a_0 \in \mathbb{R}$.

Well–posedness implies nonsingularity?

If the converse proposition holds, it is equivalent to

$$\text{well–posedness} \quad \Rightarrow \quad A \text{ nonsingular}$$

Each SAT term has rank 1: by subadditivity we get

$$\begin{aligned} rk\,(A) \leq rk\,(D_2) &+ rk\left(\alpha_0 P^{-1} E_0\,(a_0 I + b_0 S)\right) \\ &+ rk\left(\alpha_N P^{-1} E_N\,(a_1 I + b_1 S)\right) = rk\,(D_2) + 2. \end{aligned}$$

Therefore

$$rk\,(D_2) < N - 1 \quad \Rightarrow \quad A \text{ singular} \;\; \forall a_0, a_1, b_0, b_1 \in \mathbb{R}.$$

However, even by assuming $rk\,(D_2) = N-1$, we cannot conclude that A is nonsingular $(rk\,(A) \leq N+1)$. We need:

Assumption

The matrix P is diagonal. Moreover, the matrix $D_{2,CEN} \in \mathbb{R}^{(N-1)\times(N+1)}$ such that

$$D_2 = \begin{bmatrix} \mathbf{d}_{20} \\ D_{2,CEN} \\ \mathbf{d}_{2N} \end{bmatrix} \in \mathbb{R}^{(N+1)\times(N+1)}$$

has full rank.

Theorem : well–posedness $\Rightarrow$ A nonsingular

Idea of the proof:

- If P is diagonal, then the SAT terms consist of only one nonzero row each.
- It can be shown that

$$det\left(A\right) = det\begin{bmatrix} -\left[\alpha_0 P^{-1} E_0 \left(a_0 I + b_0 S\right)\right]_{0,\cdot} \\ D_{2,CEN} \\ \left[\alpha_N P^{-1} E_N \left(a_1 I + b_1 S\right)\right]_{N,\cdot} \end{bmatrix}$$

where $\left[B\right]_{i,\cdot}$ indicates the i–th row of the matrix B.

Thanks for the attention!

Short bibliography

- M. Svärd, J. Nordström, *Review of Summation-By-Parts Schemes for Initial-Boundary-Value Problems*, Journal of Computational Physics, Volume 268, pp. 1738, 2014
- N. Loehr, *Advanced Linear Algebra*, Chapman and Hall/CRC, 1st edition, 2014.
- M. H. Carpenter, D. Gottlieb, S. Abarbanel, *Time-stable boundary conditions for finite-difference schemes solving hyperbolic systems: Methodology and application to high-order compact schemes*, Journal of Comput. Physics, Vol 111 No. 2, 1994.

Remarks (ill–posedness implies singularity)

- This result does not depend on the discretization: we only need accurate operators and penalty terms.

- More generally, let $K_0, K_N \in \mathbb{R}^{(N+1)\times(N+1)}$ with the first and last column nonzero, respectively. Then

$$A = D_2 + K_0 E_0 \left(a_0 I + b_0 S\right) + K_N E_N \left(a_1 I + b_1 S\right),$$

is singular whenever (1) is satisfied.

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