

Scientific Computing

Partial Differential Equations

Jacobi Method

An iterative method to solve linear systems of equations $Ax = b$ with $A \in \mathbb{R}^{N \times N}$, $b \in \mathbb{R}^N$ is given by the Jacobi method. Starting from an initial vector $x^{(0)}$, the iteration procedure reads:

$$x_i^{(n+1)} = \frac{1}{A_{ii}} \left(b_i - \sum_{j \neq i} A_{ij} x_j^{(n)} \right), \quad i = 1, \dots, N$$

Convergence of the Jacobi Method: Diagonal dominance

A matrix $A \in \mathbb{R}^{N \times N}$ is *diagonally dominant* if the following inequality holds for all $i \in \{1, \dots, N\}$:

$$|A_{ii}| \geq \sum_{j \neq i} |A_{ij}| \quad (1)$$

Diagonal dominance is an important property of matrices and helps to show that for example the Jacobi iteration scheme for $Ax = b$ converges:

- If A is strictly diagonally dominant, that is we have a “>” in Eq. (1) for all rows i , then the Jacobi iteration converges.
- Let A be diagonally dominant and have at least one row with “>” in Eq. (1). If A is irreducible, then the Jacobi method converges.

We do not want to dive deeper into mathematics here and thus will not completely define what irreducibility means (we may discuss the respective definition during the exercise class). However, it should be noted that a matrix is irreducible if the matrix is tridiagonal and only has non-vanishing main- and subdiagonal entries, that is

$$A_{ij} \neq 0 \quad \forall |i - j| \leq 1.$$

Exercise 17: Convection-Diffusion Systems

Consider the one-dimensional differential equation

$$-\frac{d^2u(x)}{dx^2} + v \cdot \frac{du(x)}{dx} = f(x), \quad x \in (0, 1) \quad (2)$$

with velocity $v \in \mathbb{R}$ and Dirichlet boundary conditions $u(0) = c_0, u(1) = c_1$.

This equation models the transport of a quantity u in a fluid when the fluid is assumed to move at constant velocity v .

(a) Set up a *finite difference* scheme using

- the standard second-order discretisation of the diffusive term (that is the second-order derivative)
- a symmetric second-order discretisation for the convective term (that is the first-order derivative).

Write down the formulation for a single row of the arising linear system of equations

$$\sum_j A_{ij}u_j = b_i$$

with $u_j := u(j \cdot h)$, meshsize h and right-hand side b_i .

- (b) Formulate the Jacobi relaxation to solve this system. Under which conditions does the Jacobi method converge?
- (c) Replace the second-order discretisation of the first-order derivative by a first-order one-sided discretisation. Re-formulate the Jacobi relaxation for this case. Under which conditions can we expect convergence now?

Solution:

(a) The second-order stencil for the second-order derivative reads

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

and for the first-order derivative

$$\frac{du}{dx} \approx \frac{u_{i+1} - u_{i-1}}{2h}.$$

Using these approximations and defining $f_i := f(ih)$ yields:

$$\left(-1 + \frac{vh}{2}\right) u_{i+1} + 2u_i + \left(-1 - \frac{vh}{2}\right) u_{i-1} = h^2 f_i$$

At the left or right boundary, the value $u_{i-1} = u(0) = c_0$ or $u_{i+1} = u(1) = c_1$ is already known and can thus be removed from the equation for the first inner point. The

equations for the left/ right boundary read:

$$\text{Left boundary : } \left(-1 + \frac{vh}{2}\right) u_{i+1} + 2u_i = h^2 f_i - \left(-1 - \frac{vh}{2}\right) c_0$$

$$\text{Right boundary : } 2u_i + \left(-1 - \frac{vh}{2}\right) u_{i-1} = h^2 f_i - \left(-1 + \frac{vh}{2}\right) c_1$$

Our matrix A hence has the following form:

$$A_{kl} = \begin{cases} \left(-1 + \frac{vh}{2}\right) & l = k + 1 \\ 2 & \text{for } l = k \\ \left(-1 - \frac{vh}{2}\right) & l = k - 1 \end{cases}$$

The system is tridiagonal.

(b) The Jacobi iteration in iteration $n + 1$ is given by:

$$u_i^{n+1} = \frac{1}{2} \left(h^2 f_i - \left(-1 - \frac{vh}{2}\right) u_{i-1}^n - \left(-1 + \frac{vh}{2}\right) u_{i+1}^n \right)$$

where u_i^n denotes the solution in iteration n .

The condition for the diagonal dominance reads:

$$\left| -1 + \frac{hv}{2} \right| + \left| -1 - \frac{hv}{2} \right| \leq 2 \Leftrightarrow \left| \frac{vh}{2} - 1 \right| + \left| 1 + \frac{vh}{2} \right| \leq 2$$

The arising conditions for diagonal dominance at the boundaries read:

$$\text{Left boundary : } \left| \frac{vh}{2} - 1 \right| \leq 2$$

$$\text{Right boundary : } \left| -\frac{vh}{2} - 1 \right| \leq 2 \Leftrightarrow \left| \frac{vh}{2} + 1 \right| \leq 2$$

The form of the Jacobi iteration does not need to be modified at the boundaries: we only solve the linear system for the *inner* points, as there is no separate equation for the boundary points. We can now think of the different cases (to evaluate the absolute values from the inequalities above):

- For $-\infty < vh \leq -2$:

$$\text{Inner: } -\left(\frac{vh}{2} - 1\right) - \left(\frac{vh}{2} + 1\right) \stackrel{?}{\leq} 2 \Leftrightarrow vh \geq -2$$

$$\text{Left boundary: } -\left(\frac{vh}{2} - 1\right) \stackrel{?}{\leq} 2 \Leftrightarrow vh \geq -2$$

$$\text{Right boundary: } -\left(\frac{vh}{2} + 1\right) \stackrel{?}{\leq} 2 \Leftrightarrow vh \geq -6$$

where all conditions are solely fulfilled if $vh = -2$. In this case, all lower subdiagonal entries of the matrix A become zero. The matrix is hence reducible and no convergence can be proven.

- For $-2 < vh \leq 2$:

$$\text{Inner:} \quad -\left(\frac{vh}{2} - 1\right) + \left(\frac{vh}{2} + 1\right) \stackrel{?}{\leq} 2 \quad \Leftrightarrow \quad 2 \leq 2$$

$$\text{Left boundary:} \quad -\left(\frac{vh}{2} - 1\right) \stackrel{?}{\leq} 2 \quad \Leftrightarrow \quad vh \geq -2$$

$$\text{Right boundary:} \quad \left(\frac{vh}{2} + 1\right) \stackrel{?}{\leq} 2 \quad \Leftrightarrow \quad vh \leq 2$$

The equation for the left boundary is even fulfilled with $vh > -2$. If $vh = 2$, all upper subdiagonal entries are zero and the matrix becomes reducible. The convergence of Jacobi can hence be proven for $-2 < vh < 2$.

- For $2 < vh < \infty$:

$$\text{Inner:} \quad \left(\frac{vh}{2} - 1\right) + \left(\frac{vh}{2} + 1\right) \stackrel{?}{\leq} 2 \quad \Leftrightarrow \quad vh \stackrel{!}{\leq} 2$$

$$\text{Left boundary:} \quad \left(\frac{vh}{2} - 1\right) \stackrel{?}{\leq} 2 \quad \Leftrightarrow \quad vh \leq 6$$

$$\text{Right boundary:} \quad \left(\frac{vh}{2} + 1\right) \stackrel{?}{\leq} 2 \quad \Leftrightarrow \quad vh \stackrel{!}{\leq} 2$$

The inequality for the non-boundary equations and the right boundary equation cannot be fulfilled. No convergence can hence be proven for this case.

(c) We will only consider the discretisation

$$\frac{du}{dx} \approx \frac{u_{i+1} - u_i}{h}.$$

The equation system in this case evolves to be:

$$\text{Inner:} \quad (-1 + hv)u_{i+1} + (2 - hv)u_i + (-1)u_{i-1} = h^2 f_i$$

$$\text{Left boundary:} \quad (-1 + hv)u_{i+1} + (2 - hv)u_i = h^2 f_i - (-1)c_0$$

$$\text{Right boundary:} \quad (2 - hv)u_i + (-1)u_{i-1} = h^2 f_i - (-1 + hv)c_1$$

The Jacobi relaxation for this linear system of equations (for the inner points) is given by:

$$u_i^{n+1} = \frac{1}{(2 - hv)} (h^2 f_i - (-1 + hv)u_{i+1}^n - (-1)u_{i-1}^n)$$

The conditions for diagonal dominance in this case read:

$$\text{Inner:} \quad |hv - 1| + 1 \leq |vh - 2|$$

$$\text{Left boundary:} \quad |hv - 1| \leq |vh - 2|$$

$$\text{Right boundary:} \quad 1 \leq |vh - 2|$$

We can again consider different cases for v :

- $-\infty < vh \leq 1$:

$$\text{Inner:} \quad -(hv - 1) + 1 \stackrel{?}{\leq} -(vh - 2) \Leftrightarrow 0 \leq 0$$

$$\text{Left boundary:} \quad -(hv - 1) \stackrel{?}{\leq} -(vh - 2) \Leftrightarrow 0 \leq 1$$

$$\text{Right boundary:} \quad 1 \stackrel{?}{\leq} -(vh - 2) \Leftrightarrow vh \leq 1$$

All inequalities are fulfilled and the inequality for the left boundary is even fulfilled for " $<$ ". We thus obtain convergence of the Jacobi relaxation over a very wide range of vh , that is for $vh \in (-\infty, 1)$.

- $1 < vh \leq 2$:

$$\text{Inner:} \quad (hv - 1) + 1 \stackrel{?}{\leq} -(vh - 2) \Leftrightarrow vh \stackrel{!}{\leq} 1$$

$$\text{Left boundary:} \quad (hv - 1) \stackrel{?}{\leq} -(vh - 2) \Leftrightarrow vh \leq \frac{3}{2}$$

$$\text{Right boundary:} \quad 1 \stackrel{?}{\leq} -(vh - 2) \Leftrightarrow vh \stackrel{!}{\leq} 1$$

The conditions for the points in the inner part of the domain and the point near the right boundary cannot be fulfilled. We can hence not conclude convergence.

- $2 < vh < \infty$:

$$\text{Inner:} \quad (hv - 1) + 1 \stackrel{?}{\leq} (vh - 2) \Leftrightarrow 0 \stackrel{!}{\leq} -2$$

$$\text{Left boundary:} \quad (hv - 1) \stackrel{?}{\leq} (vh - 2) \Leftrightarrow 0 \stackrel{!}{\leq} -1$$

$$\text{Right boundary:} \quad 1 \stackrel{?}{\leq} (vh - 2) \Leftrightarrow vh \geq 3$$

The conditions for points in the inner part of the domain and the left boundary cannot be fulfilled. We can hence not conclude convergence.

Remarks:

- We see that the first-order discretisation of the convective term yields a larger range of velocities v for which the Jacobi method must converge. If we have to deal with velocities $v > 0$, we can apply the one-sided difference

$$\frac{du}{dx} \approx \frac{u_i - u_{i-1}}{h}$$

instead of the one from above and obtain similar results.

- From the worksheet, we only know the direction "If A is irreducible and diagonally dominant, then we have convergence". This does not imply that the Jacobi method will definitely not converge for all other cases. More analysis is required for those cases. One may for example analyse the iteration matrix of the Jacobi method and check whether its eigenvalues are within the range $(-1, 1)$.

- The conditions that we derived for the Jacobi iteration to converge can also be considered from a more general point of view: assume that the signs of the subdiagonal entries in a single row of our tridiagonal matrix A and the sign of the corresponding diagonal entry are different (for example, $A_{ii} = 2$, $A_{ii-1} = -1$, $A_{ii+1} = -1$). If both values $x_{i-1}^{(n)}$, $x_{i+1}^{(n)}$ are greater/ smaller than zero, then the value $x_i^{(n+1)}$ is greater/ smaller than zero as well (if we don't take the right-hand side b_i into consideration at this point). In this context, the method preserves positivity.

Exercise 18: Runge-Kutta for the Heat Equation

The following partial differential equation describes the distribution of the temperature T in a stick:

$$\frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial x^2}, \quad x \in (0, 1)$$

The constant D is the thermal diffusivity and describes how fast the temperature can diffuse within the stick. We further assume that the temperature of the stick at the outer ends is known, that is $T(t, x = 0) = T_0$, $T(t, x = 1) = T_N$.

- Review from the lecture: Apply the symmetric finite difference approximation for the second-order spatial derivative similar to exercise 17(a). Which kind of differential equations remains?
- Discretise the new differential equations from (a) using the method of Heun.
- Write a maple sheet that solves the discrete problem with $D = 1$, a time step $\tau = 0.001$, an initial temperature distribution $T(t = 0, x) = 0$ in the inner part of the stick and temperature values $T_0 = 0$, $T_1 = 1$. Use a mesh sizes $h = 1/20$ for the spatial discretisation and plot the result after 1, 10, 100 and 1000 time steps.

Solution:

- We introduce $N + 1$ grid points along the stick and a meshsize $h := \frac{1}{N}$. At each point $x_i := i \cdot h$, we define a temperature value $T_i(t) := T(t, x_i)$. Evaluating the partial differential equation in each point x_i and using the symmetric second-order approximation for the second-order derivative yields

$$\frac{dT_i(t)}{dt} = D \cdot \frac{T_{i+1}(t) - 2T_i(t) + T_{i-1}(t)}{h^2}, \quad i = 1, \dots, N - 1 \quad (3)$$

with T_0 and T_N prescribed at the outer boundary points as assumed in this exercise. We hence obtain a *system of ordinary differential equations* for the local temperature values $T_i(t)$ in the inner part of the domain.

(b) We introduce a matrix $A \in \mathbb{R}^{N-1 \times N-1}$ and a vector $b \in \mathbb{R}^{N-1}$:

$$A = \frac{D}{h^2} \begin{pmatrix} -2 & 1 & 0 & \dots & \dots & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ 0 & \dots & \dots & 0 & 1 & -2 & 1 \\ 0 & \dots & \dots & \dots & 0 & 1 & -2 \end{pmatrix}, \quad b = \frac{D}{h^2} \begin{pmatrix} T_0(t) \\ 0 \\ \vdots \\ 0 \\ T_N(t) \end{pmatrix} = \frac{D}{h^2} \begin{pmatrix} T_0 \\ 0 \\ \vdots \\ 0 \\ T_N \end{pmatrix}$$

Using A and b , we can write the system of ODEs from Eq. (3) as follows:

$$\frac{d}{dt} \begin{pmatrix} T_1(t) \\ \vdots \\ T_{N-1}(t) \end{pmatrix} = A \cdot \begin{pmatrix} T_1(t) \\ \vdots \\ T_{N-1}(t) \end{pmatrix} + b$$

Let's define a time step τ and the vector $\vec{T}^n := (T_1(n\tau), \dots, T_{N-1}(n\tau))^T$. Plugging in the method of Heun (see for example the slides 05_ode_numerics.pdf) for the system of ordinary differential equations from above yields:

$$\begin{aligned} \vec{T}_I^n &= \vec{T}^n \\ \vec{T}_{II}^n &= \vec{T}^n + \tau (A\vec{T}_I^n + b) \\ &= \vec{T}^n + \tau (A\vec{T}^n + b) \\ \vec{T}^{n+1} &= \vec{T}^n + \frac{\tau}{2} (A\vec{T}_I^n + b + A\vec{T}_{II}^n + b) \\ &= \vec{T}^n + \frac{\tau}{2} (A\vec{T}^n + b + A(\vec{T}^n + \tau (A\vec{T}^n + b)) + b) \\ &= \dots \\ &= \vec{T}^n + \tau (A\vec{T}^n + b) + \frac{\tau^2}{2} A (A\vec{T}^n + b) \end{aligned}$$

(c) See ws8.18c.mw. From the latter formula, we see that we need at least two vectors: one vector to store the temperature \vec{T}^n for one time step and another vector to store $A\vec{T}^n + b$. All the rows of the matrix A —except for the very first and last row—are identical. We hence do not need to store the matrix explicitly, but can apply the respective matrix entries directly! Since the storage of matrices may require huge amounts of memory, matrix-free computations should be preferred in most cases. The latter vector is denoted as *rhsvec* in the maple sheet. After the initialisation of all parameters and the vectors, we do the following steps per time step:

- Compute $A\vec{T}^n + b$. We split this computation into the evaluation close the boundaries and the inner part of the computational domain. Alternatively, one could

enlarge \vec{T}^n by two entries (one at the very beginning and one entry at the very end) which contain the boundary values. Then, we can apply the inner stencil for all entries with one loop and do not have to use the separate boundary rules.

- Compute the new temperature values. Similar to the case of the vector *rhsvec*, we have modified matrix-vector products for the points close to the boundary.

We finally obtain (after 1000 time steps) an approx. linear distribution of the temperature in the stick.