Jacobs University Bremen **Spring Semester 2016**
Prof. Dr. T. Preusser

Nonlinear Dynamics Lab

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Finite difference discretization of 1D steady state heat equation. Diffusion is a physical process, which leads to the equilibration of entities and thus to the homogeneous mixture of substances like atoms, molecules or charged particles. The diffusion is caused by the random thermal movement of the entities and the fact that a heterogeneous distribution will statistically lead to a motion of the entities from areas of high concentration into areas of low concentration. Effectively this leads to a transport of the substance such that differences in the concentration are removed until complete mixture.

In the following let $\Omega \subset \mathbb{R}^n$ be a domain in which we aim at modeling diffusion. Furthermore we consider $u : \Omega \to \mathbb{R}$ to be the substance whose diffusion is considered. As described above, the diffusion process will cause a movement of the substance from areas of high concentration to areas of low concentration. The ***flux*** of the substance is modeled by ***Fick's law***

$$J = -a\nabla u, \tag{1}$$

thus, the flux J is anti-proportional to the derivative of u (i.e. the gradient ∇u; remember that the gradient points in direction of steepest ascent, i.e. from low to high concentrations). The constant of proportionality $a > 0$ is called ***diffusion coefficient***.

During diffusion the spatial distribution of the substance u will dynamically change over time. Thus we get $u = u(t, x)$ and an equation describing the temporal evolution of the substance is governed from the combination of (1) with the ***continuity equation***

$$\partial_t u = -\mathrm{div} J + f. \tag{2}$$

The continuity equation is a so called ***conservation law***, which states that a change in the amount of substance at a certain spatial point can only be caused if there is a difference between the fluxes towards that point and the fluxes away from that point or from sources or sinks. This is expressed by the divergence of the flux J and the source/sink term $f(t, x)$.

In combination of (1) and (2) yields the ***diffusion equation***:

$$\partial_t u(t,x) - \mathrm{div}(a(t,x)\nabla u(t,x)) = f(t,x) \qquad \text{for all } (t,x) \in [0,T] \times \Omega, \tag{3}$$

where $T > 0$ is some finite time until which we model the diffusion. This is a ***second order parabolic partial differential equation (PDE)*** on $\Omega \subset \mathbb{R}^n$ for whose unique solvability an initial condition

$$u(0,x) = u^{(0)}(x) \qquad \text{for all } x \in \Omega, \tag{IC}$$

is needed. Also we need one of the boundary conditions

$$u(t,x) = g(t,x) \qquad \text{for all } (t,x) \in (0,T) \times \partial\Omega, \tag{DBC}$$

$$\nabla u(t,x) \cdot \nu(x) = g(t,x) \qquad \text{for all } (t,x) \in (0,T) \times \partial\Omega, \tag{NBC}$$

where $\nu(x)$ is the outer normal to the boundary $\partial\Omega$. The condition (DBC) is called ***essential*** or ***Dirichlet*** boundary condition, whereas (NBC) is referred to as ***natural*** or ***Neumann*** boundary condition.

In the case that the diffusion coefficient a is a constant this equation reduces to

$$\partial_t u(t,x) - a\Delta u(t,x) = f(t,x) \qquad \text{for all } (t,x) \in [0,T] \times \Omega, \tag{4}$$

again with initial condition (IC) and either (DBC) or (NBC).

In this exercise we consider the steady state of the heat equation on the interval $\Omega = [-1, 1]$. This means that the time derivative in (3) or (4) vanishes and that all quantities involved do not depend on time but are considered to be in *equilibrium*. This leads us to the *second order elliptic PDEs*

$$-(a(x)u'(x))' = f(x) \qquad \text{in } [0,T] \times [-1,1], \tag{5}$$

$$-au''(x) = f(x) \qquad \text{in } [0,T] \times [-1,1]. \tag{6}$$

as the equivalents of (3) and (4).

a) Reconsider the definition of the symbols ∇, div and Δ and thus understand how to arrive at ODEs (5) and (6) from the PDEs (3) respectively (4).

b) We discretize the equations with a finite difference approach, thus introducing a grid on the interval $[-1, 1]$ having the nodes $x_i = ih - 1$, where $i = 0, \ldots, N$ and $h = 2/N$ for some $N \in \mathbb{N}$. In the following, for all quantities an index i will denote the evaluation of this quantity at x_i, e.g. $u_i = u(x_i)$ and $a_i = a(x_i)$, etc.

The derivatives in (5) and (6) are replaced by

$$v'(x_i) \approx D_i^- v := \frac{v_i - v_{i-1}}{h} \qquad \text{backward difference quotient,}$$

$$\text{or} \qquad v'(x_i) \approx D_i^+ v := \frac{v_{i+1} - v_i}{h} \qquad \text{forward difference quotient,}$$

for any function v on Ω. An approximation of the second order derivative is obtained by taking $D_i^- D_i^+ v$ or $D_i^+ D_i^- v$. Use the difference quotients to derive a system of equations for (5) and (6), which represents the differential equations at the grid nodes. Write the system in matrix form $-M\vec{u} = \vec{f}$, where $M \in \mathbb{R}^{(N+1)\times(N+1)}$ and $\vec{u}, \vec{f} \in \mathbb{R}^{N+1}$.

c) For the concrete case of equation (6), the Dirichlet boundary condition (DBC) with $g = 0$, and the settings $a = 2$, $f = 2$ compute the analytical solution $u(x)$.

Now implement the linear system from b) and modify it such that the Dirichlet boundary conditions are met automatically. For $N = 2^j$, where $j = 2, \ldots, 10$ compute the numerical solution vector $\vec{u}$ and plot it versus the analytical solution.

d) For the various N from c) compute the following errors for the numerical solution

$$E_0 := \sqrt{\frac{2}{N} \sum_{i=1}^{N} \left| \frac{u_{i-1} + u_i}{2} - u\left(\frac{x_{i-1} + x_i}{2}\right) \right|^2} \qquad L^2 - \text{error,}$$

$$E_1 := \max_{i=1\ldots N} \left| \frac{u_{i-1} + u_i}{2} - u\left(\frac{x_{i-1} + x_i}{2}\right) \right|, \qquad L^\infty - \text{error,}$$

and draw a graph that shows $\log E_0$ and $\log E_1$ versus j. The slope of the graph is the order of convergence of the numerical solution. Report the order of convergence for your implementation.

e) Repeat the discretization and implementation for the case of problem (6) with $g = 0$, $a(x) = 1$ and

$$f(x) = \begin{cases} 2 & \text{if } x < 0 \\ 0 & \text{if } x \geq 0 \end{cases}$$

implement the numerical solution. As before you are supposed to draw plots of the solution and evaluate the errors and orders of convergence.

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Finite difference discretization of the time dependent heat equation in 1D. In the first assignment sheet we have seen that the discretization of the steady state heat equation leads to a linear system $M\vec{u} = \vec{f}$, where $M \in \mathbb{R}^{(N+1)\times(N+1)}$ and $\vec{u}, \vec{f} \in \mathbb{R}^{N+1}$ and where $M = \text{tridiag}(1, -2, 1)$. Now we will consider the time-dependent heat equation (4), i.e.

$$\frac{\partial u}{\partial t}(t,x) - a\Delta u(t,x) = f(t,x) \qquad \text{for all } (t,x) \in [0,T] \times \Omega,$$

including the initial conditon (IC) and boundary condition (DBC).

We perform the same steps of the discretization as before for the steady state system, however the nodal values will depend on time, i.e. $u_i = u_i(t)$. Thus, we will again arrive at a system of equations, which however includes the time derivative at each spatial node. Denoting the vector of time-dependent nodal values with $\vec{u}(t) = (u_0(t), \ldots, u_N(t))^t$ we get

$$\frac{\partial \vec{u}}{\partial t}(t) - M\vec{u}(t) = \vec{f}(t) \qquad \text{for all } t \in [0,T]. \tag{7}$$

Let us here consider the case $f = 0$ only, i.e. the right hand side of (7) shall vanish. Then, the solution of such a system is formally given by

$$\vec{u}(t) = \exp(tM)\vec{u}^{(0)}, \tag{8}$$

where $\vec{u}^{(0)}$ is the vector of nodal values of the initial condition $u^{(0)}$. This solution involves the exponential of the matrix M, i.e. the exponential of the discretized Laplacian Δ.

For the full discretization and the numerical solution of the ODE system we also partition the time-dimension into small units of size $\tau > 0$. We define the time-discrete points $t_j = j\tau$, $j \in \mathbb{N}$ and we seek for the solution vector $\vec{u}(t_j)$ at these time points thereby using the notation $\vec{u}^{(j)} = \vec{u}(t_j)$. According to (8) we get

$$\vec{u}^{(j)} = \exp((j\tau)M)\vec{u}^{(0)} = \underbrace{\exp(\tau M)\cdots\exp(\tau M)}_{j \text{ times}}\vec{u}^{(0)}.$$

This can be evaluated recursively by the simple rule

$$\vec{u}^{(j)} = \exp(\tau M)\vec{u}^{(j-1)} \qquad \text{for } j = 1, 2, \ldots, \tag{9}$$

for whose numerical evaluation an approximation of $\exp(\tau M)$ is needed. To this end, it is popular to use rational functions, i.e. $\exp(y) \approx \frac{Q(y)}{R(y)}$. Applied to the matrix valued exp function and in (9) we get

$$R(\tau M)\vec{u}^{(j)} = Q(\tau M)\vec{u}^{(j-1)} \qquad \text{or} \qquad \vec{u}^{(j)} = (R(\tau M))^{-1}Q(\tau M)\vec{u}^{(j-1)}.$$

In this approximation the numerator $Q(\tau M)$ is called the *explicit* part of the discretization and the denominator $R(\tau M)$ is called the *implicit* part. The explicit part only results in a matrix multiplication and thus is computationally simple and easy, the implicit part always comes with the inversion of R and thus is more complicated and computationally more cumbersome.

There are three particular choices for R and Q, which lead to well known *time stepping schemes*

$Q(y) = 1 + y,$	$R(y) = 1,$	Explicit Euler Scheme (Forward Euler),	(EE)
$Q(y) = 1,$	$R(y) = 1 - y,$	Implicit Euler Scheme (Backward Euler),	(IE)
$Q(y) = 1 + y/2,$	$R(y) = 1 - y/2,$	Crank-Nicholson Scheme.	(CN)

a) Follow the ideas of the spatial discretization and thus understand how to arrive at (8). Reconsider the definition of the exponential function for matrices.

b) On the interval $[-3, 1]$ draw graphs of the real valued exp function and its rational approximations (EE), (IE)and (CN) in order to get an impression about the approxmation.

c) It is of course wanted that the time stepping schemes converge to the true solution (7) for any starting value of the iteration. To this end, the two essential properties *consistency* (i.e. the true solution must be a fixed point of the iteration) and *stability* (i.e. small perturbations in the starting point lead to small perturbations in the result) are needed. In fact, the rational approximations are stable on the set

$$S := \left\{ y \in \mathbb{R} \;\middle|\; \left| \frac{Q(y)}{R(y)} \right| < 1 \right\}.$$

In the plot from b) draw these stability regions for the three time stepping schemes. Comment on your results.

Note that for the actual time stepping schemes considered here the eigenvalues of the matrices play the role of the y in the definition of the stability region above. In the case of the diffusion equation this condition is fulfilled *unconditionally* for (IE) and (CN). For (EE) there is a restriction on the time step $\tau < \frac{h^2}{2a}$ to arrive at a stable scheme. Thus, the (EE) method is simple as it does not require the inversion of a matrix, however as h decreases or a increases it needs smaller and smaller time-steps τ thus leading to a larger and larger computational effort.

d) Implement the three time-stepping schemes (use the matrix M you already implemented for the first exercise sheet) and try them with $\tau = 2^{-l}$ for $l = 1, \ldots, 8$, $a = 1$ and $u^{(0)}(x) = (1-x)^2(1+x)^2$. Respect the time step restriction for (EE) and compare the solutions you obtain at time $T = 0.5$.

e) For the explicit Euler scheme (EE) explicitely violate the time stepping restriction. Plot some solutions and compare them to the ones obtained from the Crank Nicholson Scheme (CN).

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Anisotropic diffusion in the two-dimensional plane. In the final assignment sheet we extend the discretization of the time-dependent diffusion equation to the two-dimensional plane and generalize the model towards anisotropic diffusion. Thus, the function u will now depend on two space variables $u = u(x, y)$ and the Laplacian $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ will be the sum of the pure second order derivatives in x and y.

Let us consider the steady state of the heat equation (4) first. For the extension of the discretization to the 2D plane we introduce a tensor product grid of the square $\Omega := [0, 1]^2$. Thus, we have nodes $x_i = ih$ and $y_j = jh$, $i, j = 0, \ldots, N$ and $h = 1/N$. As before we write $u_{ij} = u(x_i, y_j)$ for the values of the solution u at the grid nodes (x_i, y_j). The application of the finite difference operators $D^{\pm}$ in x- and y-direction yields an approximation of the Laplacian Δu:

$$\Delta u(x_i, y_j) \approx \frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}}{h^2} =: S : \begin{pmatrix} & u_{i,j-1} & \\ u_{i-1,j} & u_{ij} & u_{i+1,j} \\ & u_{i,j+1} & \end{pmatrix},$$

where the matrix S known as the *5-point stencil* of the Laplacian is given by

$$S := \frac{1}{h^2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

and where : is a scalar product on the space of square matrices defined as $A : B := \sum_{ij} A_{ij} B_{ij}$.

As before this approximation leads us to a system of equations in the unknown nodal values u_{ij} of the solution u. To this end we order the nodal values lexicographically (from top left to bottom right) in a vector in the form

$$\vec{u} = (u_{00}, \ldots, u_{N0}, u_{01}, \ldots u_{N1}, \ldots, u_{0N}, \ldots, u_{NN}) \in \mathbb{R}^{(N+1)^2}$$

and analog for the right hand side f. Then the linear system is again $-M\vec{u} = \vec{f}$ where

$$M = \frac{1}{h^2} \begin{pmatrix} -4 & 1 & * & 1 & & & & & \\ 1 & -4 & 1 & * & 1 & & & & \\ * & 1 & -4 & 1 & * & 1 & & & \\ 1 & * & 1 & -4 & 1 & * & 1 & & \\ & \ddots & & \ddots & \ddots & \ddots & & \ddots & \\ & & 1 & * & 1 & -4 & 1 & * & 1 \\ & & & 1 & * & 1 & -4 & 1 & * \\ & & & & 1 & * & 1 & -4 & 1 \\ & & & & & 1 & * & 1 & -4 \end{pmatrix} \tag{10}$$

and where $*$ stands for bands of zeros, whose width is determined by N. So M is a bandmatrix with 5 bands, i.e. 3 bands around the diagonal and two distant bands of ones, $M = \text{multidiag}(1, *, 1, -4, 1, *, 1)$.

a) Reconsider the derivation from above and understand how to arrive at the linear system of equations with matrix (10).

b) Implement this matrix vector system and test it with the right hand side $f(x, y) = 2(1 - x)x + 2(1 - y)y$ for moderate $N < 30$. Of course you will have to take care of the boundary values in a similar fashion as for the one-dimensional case.

c) Now combine the new two dimensional spatial discretization with the temporal discretization and the time-stepping schemes from the second assignment sheet. For a test you may use random initial data, i.e. just set every nodal value u_{ij}^0 to some random value in $[0, 1]$. Carefully use small enough time-steps and respect the time-step-restriction for the explicit scheme. Comment on your observation

As described in the first assignment sheet, diffusion is a process which accounts for the equilibration of concentration differences and thus causes a flux of mass (or energy) in the direction anti-proportional to the gradient. However, the material in which the diffusion takes place may not permit diffusion in this direction because it has some internal anisotropic structure (e.g. perfered directions, fibers or different layers). In this case the diffusion coefficient in (3) becomes a matrix $a(t, x) \in \mathbb{R}^{2\times 2}$ which describes the possible diffusion for every coordinate direction.

d) To model a material, which prefers diffusion in x-direction we set $a(t, x) := \begin{pmatrix} 1 & 0 \\ 0 & \varepsilon \end{pmatrix}$ for some $0 \leq \varepsilon \ll 1$. For this case perform the differentiation in (3) and find the analog of the 5-point-difference-stencil needed here.

e) Implement the linear system resulting from this discretization of the anisotropic diffusion and test it with the random initial data already used above. Use different settings for ε and see how it influences the results. Comment on your observations.

f) **Bonus assignment.** The analytical solution of the problem from b) is $u(x, y) = x(1-x)\, y(1-y)$. Analog to the error analysis from the first assignment sheet evaluate the approximation error here. To this end sum up the squared differences between numerical approximation $\vec{u}$ and the analytical solution u at the grid nodes and weight them appropriately. Create a table and draw the error values versus different grid widths h. What is the order of approximation?