Numerics of Partial Differential Equations
An Introduction - Part I

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Outline

Partial Differential Equations (PDE)

Definition

For a differential operator L which allocates a function $u:\Omega\to\mathbb{R}$, $\Omega\subseteq\mathbb{R}^d$, to

$$L[u] : \mathbb{R}^d \to \mathbb{R}\,,$$
$$u \mapsto F\Big(x, u(x), \ldots, D^\alpha u(x)\Big)\,,$$

α multiindizes, $1\leq|\alpha|\leq k$, $k\in\mathbb{N}$, and $D^\alpha := \frac{\partial^{\alpha_1}\cdots\partial^{\alpha_n}}{\partial^{|\alpha|}}$ the equation

$$L[u] = f(x)\,,\;\; f:\mathbb{R}^d\to\mathbb{R}\,,\;\; x\in\Omega\,, \tag{1}$$

is called partial differential equation (in d variables) of order k.

Partial Differential Equations

Definion

A PDE is called

- linear if F is linear in u and in all $D^\alpha u$, $1 \leq \alpha \leq k$,
- semilinear if F is linear in $D^\alpha u$, $|\alpha| = k$, and
- homogeneous if $f \equiv 0$.

Definition

A PDE of the form (1) is called well posed if

- it exists a solution u,
- the solution is unique and
- the solution depends continuously on the addition conditions.

Partial Differential Equations

Remark

There is no general procedual method for the computation of numerical solutions of alls PDEs.

Conclusion

A classification is necessary

Classification

In general the equations are classified in elliptic, parabolic and hyperbolic PDEs.

Remark

The nomenclature is arised from the cone sections.

Classification of Linear PDEs

Linear PDEs in $\mathbb{R}^2$ of Order 2

In the following we consider equations of the form

$$\sum_{i,k=1}^{2} A_{ik} u_{x_i x_k} + \sum_{i=1}^{2} B_i u_{x_i} + Cu = D\,. \qquad (2)$$

For the classification only the coefficients of the highest derivatives will be examined.

Definition

A PDE of the form (2) is called

- elliptic if $4A_{11}A_{22} - A_{12}^2 > 0$,
- parabolic if $4A_{11}A_{22} - A_{12}^2 = 0$ and
- hyperbolic if $4A_{11}A_{22} - A_{12}^2 < 0$.

Classification of Linear PDEs

Remark

- For more general PDEs the classification is defined by the eigenvalues of the coeffizient matrix.
- PDEs of order 1 are hyperbolic.
- The classification has in general only a local behavior.

Example for Local Classification

The equation $u_{xx} + u u_{yy} = 0$ is in $x \in \Omega$,

- $u(x) > 0$ elliptic,
- $u(x) = 0$ parabolic and
- $u(x) < 0$ hyperbolic.

Typical Examples

Laplace-Equation (elliptic, homogeneous, linear, order 2)

$$u_{xx} + u_{yy} = 0\,, \quad (x, y) \in \Omega \subseteq \mathbb{R}^2\,.$$

Heat-Equation (parabolic, homogeneous, linear, order 2)

$$u_t - u_{xx} = 0\,, \quad (x, t) \in [x_0, x_f] \times [t_0, t_f]\,, \;\; t_f \in (t_0, \infty]\,.$$

Wave-Equation (hyperbolic, inhomogeneous, linear, order 2)

$$u_{tt} - c^2 u_{xx} = f\,, \quad (x, t) \in [x_0, x_f] \times [t_0, t_f]\,.$$

Initial and Boundary Conditions

Remark

- A PDE has per se in general multiple solutions.
- For an unique solution additional conditions are necessary.

Samples of Boundary Conditions (BC)

For elliptic and parabolic PDEs i.a.

- Dirichlet-BC

$$u(x) = g(x)\,, \quad g : \partial\Omega \to \mathbb{R}\,, \quad x \in \partial\Omega\,, \quad or$$

- Neumann-BC:

$$\frac{\partial u}{\partial n}(x) = g(x)\,, \quad g : \partial\Omega \to \mathbb{R}\,, \quad x \in \partial\Omega\,.$$

can be applied.

Initial and Boundary Conditions

Initial Conditions

For parabolic PDEs besides BCs supplementary IC

$$u(x, t_0) = u_0(x)\,, \;\; u_0 : \Omega \rightarrow \mathbb{R}\,, \;\; x \in \Omega\,,$$

are necessary.

Cauchy-Problem

For hyperbolic PDEs besides BCs two ICs (the ordinary IC and its derivative) are necessary. A initial Cauchy-Problem has to be solved.

Dirichlet-Problem of the Poisson-Equation

Definition

Let Ω be a restricted subset of $\mathbb{R}^d$, $d \in \mathbb{N}$, and $\partial\Omega$ the corresponding boundary. Then for given functions $f : \Omega \to \mathbb{R}$ and $g : \partial\Omega \to \mathbb{R}$ the Dirichlet-Problem of the Poisson-Equation reads

$$-\sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2} u = f \quad \text{in } \Omega \,, \tag{3}$$

$$u = g \quad \text{on } \partial\Omega \tag{4}$$

with unknown function $u : \bar{\Omega} \to \mathbb{R}$.

Dirichlet-Problem of the Poisson-Equation

Notation

For $u : \Omega \subset \mathbb{R}^d \to \mathbb{R}$ we use

$$\begin{aligned} \partial_i u &:= \tfrac{\partial}{\partial x_i} u && \text{for } i = 1, \dots, d\,, \\ \partial_{ij} u &:= \tfrac{\partial^2}{\partial x_i \partial x_j} u && \text{for } i, j = 1, \dots, d\,, \\ \Delta u &:= \left(\partial_{11} + \ldots + \partial_{dd}\right) u && \text{(Laplace-Operator)}\,. \end{aligned}$$

Consequence

The Dirichlet-Problem (3)-(4) reads also

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega\,, \\ u &= g \quad \text{on } \partial\Omega\,. \end{aligned}$$

Dirichlet-Problem of the Poisson-Equation

Function Spaces

For an open subset Ω of $\mathbb{R}^d$, $d \in \mathbb{N}$, the spaces

$$C(\Omega) := \left\{ u : \Omega \to \mathbb{R} \;\middle|\; u \text{ continuous in } \Omega \right\} \quad \text{and}$$

$$C^k(\Omega) := \left\{ u \in C(\Omega) \;\middle|\; D^\alpha u \text{ exists in } \Omega \text{ for } |\alpha| \leq k \text{ and } D^\alpha u \in C(\Omega) \right\}$$

and analog $C(\bar{\Omega})$, $C^k(\bar{\Omega})$ as well as $C(\partial\Omega)$ are defined.

Definition

Let $f \in C(\Omega)$, $g \in C(\partial\Omega)$. A function u is called classical solution of the boundary problem (3)-(4) if $u \in C^2(\Omega) \cap C(\bar{\Omega})$, (3) holds for all $x \in \Omega$ and (4) for all $x \in \partial\Omega$.

Finite Difference Method (FDM)

Idea

- Compute approximations of the solution in finite discrete grid points of $\bar{\Omega}$.
- Replace the derivatives in (3) by difference quotients using only function values defined in the grid points.
- Demand (4) only in grid points.

Consequence

Generation of a linear equation system for the approximation values $\Rightarrow$ Discretization of the boundary problem

Derivative by Difference Quotients

Lemma

Let $\Omega := (x-h, x+h)$, $x \in \mathbb{R}$, $h > 0$. Then there exists a bounded $R \in \mathbb{R}$ such that

1. for $u \in C^2(\bar{\Omega})$: $\quad u'(x) = \frac{u(x+h)-u(x)}{h} + hR, \qquad |R| \leq \frac{1}{2}\|u''\|_\infty$
   forward difference quotient
2. for $u \in C^2(\bar{\Omega})$: $\quad u'(x) = \frac{u(x)-u(x-h)}{h} + hR, \qquad |R| \leq \frac{1}{2}\|u''\|_\infty$
   backward difference quotient
3. for $u \in C^3(\bar{\Omega})$: $\quad u'(x) = \frac{u(x+h)-u(x-h)}{2h} + h^2 R, \quad |R| \leq \frac{1}{6}\|u'''\|_\infty$
   central difference quotient
4. for $u \in C^4(\bar{\Omega})$: $\quad u''(x) = \frac{u(x+h)-2u(x)+u(x-h)}{h^2} + h^2 R,$
   $|R| \leq \frac{1}{12}\|u^{(4)}\|_\infty$

Proof

Generation of the Grid

Remark

In the following the domain is defined by the rectangle

$$\Omega = (0, a) \times (0, b).$$

Parameter h defines the discretization parameter with assigns particularly the dimension of the discrete problem. For an equidistant step size it holds

$$a = lh \quad b = mh \quad \text{for some } l, m \in \mathbb{N}.$$

Generation of the Grid

Discrete grid points

The grid points in Ω are defined by

$$\Omega_h := \Big\{(ih, jh) \,\Big|\, i=1,\dots,l-1,\ j=1,\dots,m-1\Big\}$$
$$= \Big\{(x,y)\in\Omega \,\Big|\, x=ih,\ y=jh \text{ with } i,j\in\mathbb{Z}\Big\}$$

and the grid points on $\partial\Omega$ by

$$\partial\Omega_h := \Big\{(ih, jh) \,\Big|\, i\in\{0,l\},\ j\in\{0,\dots,m\} \text{ oder } i\in\{0,\dots,l\},\ j\in\{0,m\}\Big\}$$
$$= \Big\{(x,y)\in\partial\Omega \,\Big|\, x=ih,\ y=jh \text{ with } i,j\in\mathbb{Z}\Big\}.$$

The collectivity of the grid points is denoted by $\bar{\Omega}_h := \Omega_h \cup \partial\Omega_h$.

Assembling of the Linear System

Discretization

Applying of this approximation to the boundary problem (3)-(4) leads in each grid point $(ih, jh) \in \Omega_h$ under disregarding of the terms Rh^2 to

$$-\left(\frac{u((i+1)h, jh) - 2u(ih, jh) + u((i-1)h, jh)}{h^2} + \frac{u(ih, (j+1)h) - 2u(ih, jh) + u(ih, (j-1)h)}{h^2}\right) = f(ih, jh)\,.$$

For the grid points on the boundary $\partial\Omega_h$ no approximation are necessary. The values are defined directly by

$$u(ih, jh) = g(ih, jh)\,.$$

Assembling of the Linear System

System of equations

After an easy converting and under using of a short notation the corresponding linear system of equations is defined for $i=1,\ldots,l-1$, $j=1,\ldots,m-1$ by the typical 5-point-stencil

$$\frac{1}{h^2}\left(-u_{i,j-1}-u_{i-1,j}+4u_{i,j}-u_{i+1,j}-u_{i,j+1}\right) = f_{i,j}$$

and for $i\in\{0,l\}$, $j=0,\ldots,m$ and $i=0,\ldots,l$, $j\in\{0,m\}$ by

$$u_{i,j} := u(ih,jh) = g(ih,jh) =: g_{ij}\,.$$

Dimension

After an adequate numering of the grid points the system above can be written as $\tilde{A}_h u_h = \tilde{q}_h$, $\tilde{A}_h \in \mathbb{R}^{M,M}$, $M=(l+1)(m+1)$.

Discrete System Matrix

Definition

A grid point $(x, y) \in \Omega_h$ is called close to the boundary if at least one of it's direct neighbors is on $\partial\Omega$.

Simplification

In case of the grid points close to the boundary the values of the neighbors $u \in \partial\Omega$ can be moved to the right hand side such that the linear system of equations reads

$$A_h u_h = q_h\,,\ A_h \in \mathbb{R}^{M_1, M_1},\ u_h, q_h \in \mathbb{R}^{M_1},\ M_1 = (l-1)(m-1).$$

Numbering

An obvious numbering is the so called lexicographical line by line counting.

Discrete System Matrix

System Matrix

$$A_h = \frac{1}{h^2}\begin{pmatrix} T & -I & & & \\ -I & T & -I & & \\ & \ddots & \ddots & \ddots & \\ & & -I & T & -I \\ & & & -I & T \end{pmatrix}, T = \begin{pmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 4 \end{pmatrix},$$

$T, I \in \mathbb{R}^{l-1,l-1}$.

Discrete Right Hand Side

Right Hand Side (RHS)

As a result of the elimination process the rhs is defined by

$$q_h = -\hat{A}_h g + f$$

with $g \in \mathbb{R}^{M_2}$, $M_2 = 2(l+m)$, $f \in \mathbb{R}^{M_1}$ and $\hat{A}_h \in \mathbb{R}^{M_1, M_2}$,

$$(\hat{A}_h)_{ij} = \begin{cases} -\frac{1}{h^2} & \text{if node } i \text{ is close to the boundary and } j \text{ is a neighbour in the 5-point-stancel and on } \partial\Omega \\ 0 & \text{otherwise} \end{cases} .$$

Discretization Error of the FDM

Definition

Let $u : \Omega \to \mathbb{R}$ be the continuous solution of the PDE and $u_h : \Omega_h \to \mathbb{R}$ the discrete solution of the corresponding linear system. Then the discretization error is defined by

$$\left\| U - u_h \right\|$$

with grid function

$$\begin{aligned} U : \Omega_h &\to \mathbb{R}, \\ x &\mapsto U(ih, jh) := u(ih, jh) \end{aligned}$$

and an adequate norm $\|.\|$.

Norm

Definition

We are looking for a norm $\|.\|_h$ for which the discretization method converges in the sence that

$$\left\|u_h - u_h\right\|_h \to 0 \quad \text{for} \quad h \to 0$$

holds or that even the convergence rate $p > 0$ exists such that

$$\left\|u_h - U\right\|_h \leq Ch^p$$

is fullfilled.

Examples

Adequate norms are e.g. $\|.\|_\infty$ and $\|.\|_{0,h}$.

Finite Difference Method

Drawbacks

- Unnatural high smoothness capacity (Taylor).
- Approaches of higher order!?
- Complicated handling for polynomial bounded domains.

Thank you for your attention!

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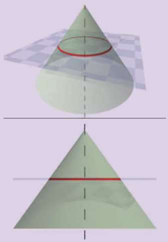
The Cone Sections

Circle



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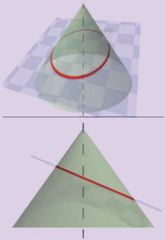
Ellipse



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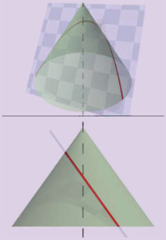
Parabola



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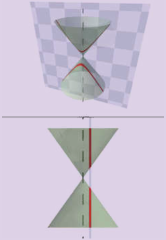
Hyperbola



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Remark

In the cartesian coordinate system the (nonemply) graph of a quadratic equation is always located by a cone section.

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The Taylor Series

Lemma

The Taylor series of a function $f(x)$ that is infinity differentiable in a neighbourhood of a is the power series

$$\sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n \,.$$

In case of a $(k+1)$ times differentiable function the series can written by

$$\sum_{n=0}^{k} \frac{f^{(n)}(a)}{n!}(x-a)^n + R_n(x)$$

with

$$R_n(x) = \int_a^x \frac{(x-t)^k}{k!} f^{(k+1)}(t)dt \,.$$

back

First Derivative by Difference Quotients

Proof

Let $u \in C^2(\bar{\Omega})$, $\Omega := (x-h, x+h)$, $x \in \mathbb{R}$, $h > 0$. Then the Taylor formula provides

$$u(x-h) = u(x) - hu'(x) + \frac{h}{2}u''(x-\xi_-)\,, \quad \xi_- \in [0,h]\,,$$

and

$$u(x+h) = u(x) + hu'(x) + \frac{h}{2}u''(x+\xi_+)\,, \quad \xi_+ \in [0,h]\,,$$

and with it directly the first two assertions. Substraction of both equations leads furthermore for $u \in C^3(\bar{\Omega})$ to the central difference quotient.

Second Derivative by Difference Quotients

Proof

The Taylor formula offers for $u \in C^4(\bar{\Omega})$ similarly

$$u(x-h) = u(x) - hu'(x) + \frac{h}{2}u''(x) - \frac{h}{6}u'''(x) + \frac{h}{24}u^{(4)}(x-\xi_-)$$

with a $\xi_- \in [0, h]$ and

$$u(x+h) = u(x) + hu'(x) + \frac{h}{2}u''(x) + \frac{h}{6}u'''(x) + \frac{h}{24}u^{(4)}(x+\xi_-)$$

for $\xi_+ \in [0, h]$. An addition of both equations leads after all to the approximation of the second derivative.

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