5.8 Unstructured domain discretization

Finite Difference discretization methods demand high regularity conditions and are best suited for structured domains (e.g., image processing). On unstructured computational domains, e.g., neuron morphologies, there is a better approach. The key idea of *Finite Element* methods is to approximate the function space instead of the differential operators. The solution space depends on the boundary value problem and needs to be chosen correctly, in order to guarantee existence and uniqueness of the solution. This requires some background in functional analysis.

Short excursion into functional analysis

Definition 6. $\|.\|_U$ *is a* norm *on a vector space* U*, if*

$$\begin{aligned} \|u+v\|_U &\leq \|u\|_U + \|v\|_U && \forall u, v \in U \\ \|\lambda u\|_U &= |\lambda| \|u\|_U && \forall u \in U, \lambda \in \mathbb{R} \\ \|u\|_U &> 0 && \forall 0 \neq u \in U \end{aligned}$$

Definition 7. $\langle \cdot, \cdot \rangle$ *is a* scalar product *on* $U \times U$*, if*

$$\begin{aligned} \langle u + \lambda v, w \rangle_U &= \langle u, w \rangle_U + \lambda \langle v, w \rangle_U \\ \langle u, v \rangle_U &= \langle v, u \rangle_U \\ \langle u, u \rangle &> 0 \end{aligned}$$

Definition 8. *(Matrix norms)*
Let U, V *be vector spaces with norms* $\| \cdot \|_U$ *and* $\| \cdot \|_F$*. The matrix norm for a mapping* $A : U \to F$ *is*

$$\|A\|_{F \leftarrow U} := \sup_{0 \neq u \in U} \frac{\|A\|_F}{\|u\|_U}.$$

With this definition we get $\|Au\|_F \leq \|A\|_{F \leftarrow U} \|u\|_U$. Matrix norms are sub-multiplicative, i.e., for $(U, \| \cdot \|_U), (V, \| \cdot \|_V), (W, \| \cdot \|_W)$ and $A : V \to W, B : U \to V$ it follows

$$\|AB\|_{W \leftarrow U} \leq \|A\|_{W \leftarrow V} \|B\|_{V \leftarrow U}.$$

Definition 9. *The* spectral radius *is defined as*

$$\varrho(A) = \max_i |\lambda_i|,$$

λ_i *being the eigenvalues of* A*.*

If A is normal, i.e., $AA^T = A^T A$, then $\varrho(A) = \|A\|_{U \leftarrow U}$. The *spectral norm* $\| \cdot \|_{U \leftarrow U}$ is the matrix norm associated with the Euclidian norm

$$\|u\|_U = \sqrt{c \sum_{i=1}^{n} |u_i|^2}.$$

Continuous functions

Let $\Omega \subset \mathbb{R}^d$ open, with closure $\bar{\Omega}$. The linear space of continuous functions $\Omega \to \mathbb{R}^m$ or $\mathbb{C}^m$ is denoted by $C(\Omega, \mathbb{R}^m)$ or $C(\Omega)$. Partial derivatives can be written as $D^\nu u(x)$, where $\nu = (\nu_1, \ldots, \nu_d)$, $\nu_i \geq 0$ is a multi-index of length $|\nu| = \nu_1 + \ldots + \nu_d$. Then

$$D^\nu = \left(\frac{\partial}{\partial x_1}\right)^{\nu_1} \cdots \left(\frac{\partial}{\partial x_d}\right)^{\nu_d}.$$

If $k = |\nu|$, then D^ν is a derivative of order k. The space of k-times differentiable functions is $C^k(\Omega) = \{u : D^\nu u \text{ exists and belongs to } C(\Omega), \forall |\nu| \leq k\}$. Functions with finite norm $\|u\|_{C^k(\Omega)} = \|u\|_{C^k} := \sup\{|D^\nu u(x)|_\infty : |\nu| \leq k, x \in \Omega\}$ form the subset

$$\bar{C}^k(\Omega) = \{u \in C^k(\Omega) : \|u\|_{C^k} < \infty\}.$$

Normed spaces A space U equipped with a norm $(U, \|\cdot\|_U)$ is a normed space.

Banach spaces A Banach space is a *complete* and *normed space*. A space is called complete, if every Cauchy-series converges to a limit contained in the space. For example, $(\bar{C}^k(\Omega), \|\cdot\|_{C^k})$ is a Banach space.

Hilbert spaces Banach spaces equipped with a scalar product is Hilbert space. For finite element theory we will make use of special Hilbert spaces.

Sobolev spaces

With $L^p(\Omega)$ or $L^p(\Omega, \mathbb{R}^m), 1 \leq p < \infty$, we denote the measurable functions with finite norm

$$\|u\|_{L^p(\Omega)} = \|u\|_{L^p} = \left(\int_\Omega |u(x)|_p^p dx\right)^{1/p},$$

with

$$|v|_p = \left(\sum_{i=1}^m |v_i|^p\right)^{1/p}.$$

$L^p(\Omega)$ is a Banach space for $p \in [1, \infty[$ and a Hilbert space for $p = 2$. For $p = 2$ we write the scalar product

$$(u, v)_{L^p(\Omega)} = \int_\Omega \sum_{i=1}^m u_i(x) v_i(x), \quad u, v \in L^2(\Omega, \mathbb{R}^m).$$

Weak differentiability

In $L^2(\Omega)$ the notion of classical differentiability (point-wise) does not apply. We can "weaken" differentiability in an integral sense:
Consider integration by parts

$$\int_\Omega f'(x)\phi(x)dx = -\int_\Omega f(x)\phi'(x)dx$$

for $\phi\,|_{\partial\Omega} = 0$.

Definition 10. *If for $f \in L^2(\Omega)$ there exists a function $g \in L^2(\Omega)$, such that*

$$-\int_\Omega f'(x)\phi(x)dx = -\int_\Omega g(x)\phi(x)dx = \int_\Omega f(x)\phi'(x)dx$$

then g is called weak derivative *of f.*

Note:

1. Functions that are differentiable in the classical (strong) sense, are also weakly differentiable.

2. Sufficiently often weak differentiable functions are differentiable in the strong sense (see Sobolev's theorem later).

Definition 11. *(Higher weak differentiability)*
Let $\nu = (\nu_1, \ldots, \nu_n)$ with $|\nu| = \sum_{i=1}^n \nu_i$ and

$$D^\nu := \frac{\partial^{|\nu|}}{\partial^{\nu_1} x_1 \cdots \partial^{\nu_n} x_n}$$

and $f \in L^2(\Omega)$. Then g is the ν-th weak derivative of f, if

$$\int_\Omega g(x)\phi(x)dx = (-1)^{|\nu|}\int_\Omega f(x)D^\nu\phi(x)dx, \quad \forall\phi \in C^\infty(\Omega), \phi\,|_{\partial\Omega} = 0$$

If $D^\nu u \in L^p(\Omega), \quad \forall|\nu| \le k$, then u belongs to the Sobolev space $W^{p,k}(\Omega)$ of order k with norm

$$\|u\|_{W^{p,k}} = \left(\sum_{|\nu|\le k} \|D^\nu u\|_{L^p}^p\right)^{1/p}.$$

For $p = 2$ we write $H^k(\Omega)$ instead of $W^{2,k}(\Omega)$:

$$\begin{aligned} H^k(\Omega) &= \left\{u : D^\nu u \in L^2(\Omega), \text{ for } |\nu| \le k\right\} \\ \|u\|_{H^k(\Omega)} = \|u\|_{H^k} &:= \left(\sum_{|\nu|\le k} \|D^\nu u\|_{L^2(\Omega)}^2\right)^{1/2} \end{aligned}$$

Theorem 2. *(Sobolev embedding theorem)*

$$H^s(\mathbb{R}^n) \subset C^k(\mathbb{R}^n), \text{ if } s > k + \frac{n}{2}, k \in \mathbb{N}_0$$

Definition 12. *(Dual spaces)*
Let V be a Hilbert space. Then we denote with V' the dual space of V containing all bounded, linear functionals $V' : V \to \mathbb{R}$:

$$V' = L(V, \mathbb{R})$$

with

$$\|v'\|_{V'} = \sup\left\{\frac{|v'(v)|}{\|v\|_V} : 0 \neq v \in V\right\}$$

Theorem 3. *(Riesz theorem)*
Let V be a Hilbert space and $v' \in V'$ a linear functional. Then there exists exactly one $w \in V$, such that

$$v'(v) = (v, w)_V \quad \forall v \in V, \|v'\|_{V'} = \|w\|_{V'}.$$

Bi-linear forms

Let V be a Hilbert space with scalar product $(\cdot, \cdot)_V$ and norm $\|u\|_V = (u, u)_V^{1/2}$. The mapping $a : V \times V \to \mathbb{R}$ is called

1. *bi-linear*, if

$$\begin{aligned} a(u + \alpha v, w) &= a(u, w) + \alpha a(v, w), \quad \alpha \in \mathbb{R}, u, v, w \in V \\ a(u, v + \alpha w) &= a(u, v) + \alpha a(u, w) \end{aligned}$$

2. *bounded*, if

$$|a(u, v)| \leq C_s \|u\|_V \|v\|_V \quad (u, v \in V).$$

3. *V-elliptic*, if

$$a(v, v) \geq C_e \|v\|_V^2.$$

Lemma 2. *For a continuous bi-linear form a, there exists a unique operator $A \in L(V, V')$ with*

$$\begin{aligned} a(v, w) &= \langle Av, w \rangle_{V' \times V} \quad \forall v, w \in V \\ \|A\|_{V' \leftarrow V} &\leq C_s \end{aligned}$$

5.9 Variational formulation

The goal of this section is to use functional analysis to propose a new approach to our model problem. Formulating an equivalent problem to the classical problem is done by finding a variational formulation. Solving the variational problem in appropriate Hilbert spaces will deliver solutions of the classical problem.

Theorem 4. *(Characterization theorem)*
Let V be a linear space and

$$a : V \times V \longrightarrow \mathbb{R}$$

symmetric and positiv. Let $f : V \longrightarrow \mathbb{R}$ be a linear functional. The function

$$J(v) := \frac{1}{2} a(v, v) - f(v)$$

has a minimum in V at u, if and only if

$$a(u, v) = f(v) \quad \forall v \in V.$$

The solution u ist is unique.