

Chapter 12

Partial differential equations

12.1 Differential operators in \mathbb{R}^n

The gradient and Jacobian

We recall the definition of the *gradient* of a scalar function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, as

$$\text{grad } f = \nabla f = \left(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n} \right)^T = \frac{\partial f}{\partial x_i}, \quad (12.1)$$

in vector notation and index notation, respectively, which we can interpret as the differential operator

$$\nabla = \left(\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_n} \right)^T = \frac{\partial}{\partial x_i}, \quad (12.2)$$

acting on the function f . The *directional derivative* $\nabla_v f$, in the direction of the vector $v : \mathbb{R}^n \rightarrow \mathbb{R}^n$, is defined as

$$\nabla_v f = \nabla f \cdot v. \quad (12.3)$$

For a vector valued function $F : \mathbb{R}^n \rightarrow \mathbb{R}^m$, we define the *Jacobian* J ,

$$J = F' = \begin{bmatrix} \frac{\partial F_1}{\partial x_1} & \dots & \frac{\partial F_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_m}{\partial x_1} & \dots & \frac{\partial F_m}{\partial x_n} \end{bmatrix} = \begin{bmatrix} (\nabla F_1)^T \\ \vdots \\ (\nabla F_m)^T \end{bmatrix} = \frac{\partial F_i}{\partial x_j}. \quad (12.4)$$

Divergence and rotation

For $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ we define the *divergence*,

$$\text{div } F = \nabla \cdot F = \frac{\partial F_1}{\partial x_1} + \dots + \frac{\partial F_n}{\partial x_n} = \frac{\partial F_i}{\partial x_i}, \quad (12.5)$$

and, for $n = 3$, the *rotation*,

$$\operatorname{rot} F = \operatorname{curl} F = \nabla \times F, \quad (12.6)$$

where

$$\nabla \times F = \det \begin{bmatrix} e_1 & e_2 & e_3 \\ \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_3} \\ F_1 & F_2 & F_3 \end{bmatrix} = \left(\frac{\partial F_3}{\partial x_2} - \frac{\partial F_2}{\partial x_3}, \frac{\partial F_1}{\partial x_3} - \frac{\partial F_3}{\partial x_1}, \frac{\partial F_2}{\partial x_1} - \frac{\partial F_1}{\partial x_2} \right),$$

with $e = (e_1, e_2, e_3)$ the standard basis in \mathbb{R}^3 .

The divergence can be understood in terms of the *Gauss theorem*,

$$\int_{\Omega} \nabla \cdot F \, dx = \int_{\Gamma} F \cdot n \, ds, \quad (12.7)$$

which relates the volume integral over a domain $\Omega \subset \mathbb{R}^3$, with the surface integral over the boundary Γ with normal n .

Similarly, the rotation can be interpreted in terms of the *Kelvin-Stokes theorem*,

$$\int_{\Sigma} \nabla \times F \cdot ds = \int_{\partial \Sigma} F \cdot dr, \quad (12.8)$$

which relates the surface integral of the rotation over a surface Σ to the line integral over its boundary $\partial \Sigma$ with positive orientation defined by dr .

Laplacian and Hessian

We express the *Laplacian* Δf as,

$$\Delta f = \nabla^2 f = \nabla^T \nabla f = \nabla \cdot \nabla f = \frac{\partial^2 f}{\partial x_1^2} + \dots + \frac{\partial^2 f}{\partial x_n^2} = \frac{\partial^2 f}{\partial x_i^2}, \quad (12.9)$$

and the *Hessian* H ,

$$H = f'' = \nabla \nabla^T f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \dots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{bmatrix} = \frac{\partial^2 f}{\partial x_i \partial x_j}. \quad (12.10)$$

The *vector Laplacian* is defined as the

$$\Delta F = \nabla^2 F = (\Delta F_1, \dots, \Delta F_n), \quad (12.11)$$

and for $m = n = 3$, we have

$$\Delta F = \nabla(\nabla \cdot F) - \nabla \times (\nabla \times F). \quad (12.12)$$

Partial integration in \mathbb{R}^n

For a scalar function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, and a vector valued function $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$, we have the following generalization of partial integration over a domain $\Omega \subset \mathbb{R}^n$, referred to as *Green's theorem*,

$$(\nabla f, F)_{L^2(\Omega)} = -(f, \nabla \cdot F)_{L^2(\Omega)} + (f, F \cdot n)_{L^2(\Gamma)}, \quad (12.13)$$

with boundary Γ and outward unit normal vector $n = n(x)$ for $x \in \Gamma$, where we use the notation,

$$(v, w)_{L^2(\Omega)} = \int_{\Omega} v \cdot w \, dx, \quad (12.14)$$

for two vector valued functions v, w , and

$$(v, w)_{L^2(\Gamma)} = \int_{\Gamma} v \cdot w \, ds, \quad (12.15)$$

for the boundary integral. For two scalar valued functions the scalar product in the integrand is replaced by the usual multiplication. With $F = \nabla g$, for $g : \mathbb{R}^n \rightarrow \mathbb{R}$ a scalar function, Green's theorem gives,

$$(\nabla f, \nabla g)_{L^2(\Omega)} = -(f, \Delta g)_{L^2(\Omega)} + (f, \nabla g \cdot n)_{L^2(\Gamma)}. \quad (12.16)$$

12.2 Function spaces

The Lebesgue spaces $L^p(\Omega)$

Let Ω be a domain in \mathbb{R}^n and let p be a positive real number, then we define the *Lebesgue space* $L^p(\Omega)$ by

$$L^p(\Omega) = \{f : \|f\|_p < \infty\}, \quad (12.17)$$

with the $L^p(\Omega)$ norm,

$$\|f\|_p = \left(\int_{\Omega} |f(x)|^p \, dx \right)^{1/p}, \quad (12.18)$$

where in the case of a vector valued function $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$,

$$|f(x)|^p = |f_1(x)|^p + \dots + |f_n(x)|^p, \quad (12.19)$$

or a matrix valued function $f : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n}$,

$$|f(x)|^p = \sum_{i,j=1}^n |f_{ij}(x)|^p. \quad (12.20)$$

$L^p(\Omega)$ is a vector space, since (i) $\alpha f \in L^p(\Omega)$ for any $\alpha \in \mathbb{R}$, and (ii) $f + g \in L^p(\Omega)$ for $f, g \in L^p(\Omega)$, by the inequality,

$$(a + b)^p \leq 2^{p-1}(a^p + b^p), \quad a, b \geq 0, 1 \leq p < \infty, \quad (12.21)$$

which follows from the convexity of the function $t \mapsto t^p$.

$L^p(\Omega)$ is a Banach space, and $L^2(\Omega)$ is a Hilbert space with the inner product (12.14) which induces the $L^2(\Omega)$ -norm. In the following we let it be implicitly understood that $(\cdot, \cdot) = (\cdot, \cdot)_{L^2(\Omega)}$ and $\|\cdot\| = \|\cdot\|_{L^2(\Omega)}$.

Sobolev spaces

To construct appropriate vector spaces for variational formulations of partial differential equations, we need to extend the spaces $L^2(\Omega)$ to include also derivatives. The *Sobolev space* $H^1(\Omega)$ is defined by,

$$H^1(\Omega) = \{v \in L^2(\Omega) : \nabla v \in L^2(\Omega)\}, \quad (12.22)$$

and we define

$$H_0^1(\Omega) = \{v \in H^1(\Omega) : v(x) = 0, \forall x \in \Gamma\}, \quad (12.23)$$

to be the space of functions in $H^1(\Omega)$ that are zero on the boundary Γ .

12.3 FEM for Poisson's equation

The Poisson equation

We now consider the *Poisson equation* for an unknown function $u : \mathbb{R}^n \rightarrow \mathbb{R}$,

$$-\Delta u = f, \quad x \in \Omega, \quad (12.24)$$

with $\Omega \subset \mathbb{R}^n$, and given data $f : \mathbb{R}^n \rightarrow \mathbb{R}$. For the equation to have a unique solution we need to specify boundary conditions. We may prescribe *Dirichlet boundary conditions*,

$$u = g_D, \quad x \in \Gamma, \quad (12.25)$$

Neumann boundary conditions,

$$\nabla u \cdot n = g_N, \quad x \in \Gamma, \quad (12.26)$$

with $n = n(x)$ the outward unit normal on Γ_N , or a linear combination of the two, which we refer to as a *Robin boundary condition*.

Homogeneous Dirichlet boundary conditions

We now state the variational formulation of Poisson equation with homogeneous Dirichlet boundary conditions,

$$-\Delta u = f, \quad x \in \Omega, \quad (12.27)$$

$$u = 0, \quad x \in \Gamma, \quad (12.28)$$

which we obtain by multiplication with a test function $v \in V = H_0^1(\Omega)$ and integration over Ω . Using Green's theorem, we obtain the variational formulation: find $u \in V$, such that

$$(\nabla u, \nabla v) = (f, v), \quad (12.29)$$

for all $v \in V$, since the boundary term vanishes as the test function is an element of the vector space $H_0^1(\Omega)$.

Homogeneous Neumann boundary conditions

We now state the variational formulation of Poisson equation with homogeneous Neumann boundary conditions,

$$-\Delta u = f, \quad x \in \Omega, \quad (12.30)$$

$$\nabla u \cdot n = 0, \quad x \in \Gamma, \quad (12.31)$$

which we obtain by multiplication with a test function $v \in V = H^1(\Omega)$ and integration over Ω . Using Green's theorem, we get the variational formulation: find $u \in V$, such that,

$$(\nabla u, \nabla v) = (f, v), \quad (12.32)$$

for all $v \in V$, since the boundary term vanishes by the Neumann boundary condition. Thus the variational forms (12.29) and (12.32) are similar, with the only difference being the choice of test and trial spaces.

However, it turns out that the variational problem (12.32) has no unique solution, since for any solution $u \in V$, also $v + C$ is a solution, with $C \in \mathbb{R}$ a constant. To ensure a unique solution, we need an extra condition for the solution which determines the arbitrary constant, for example, we may change the approximation space to

$$V = \{v \in H^1(\Omega) : \int_{\Omega} v(x) dx = 0\}. \quad (12.33)$$

Non homogeneous boundary conditions

Poisson equation with non homogeneous boundary conditions takes the form,

$$-\Delta u = f, \quad x \in \Omega, \quad (12.34)$$

$$u(x) = g_D, \quad x \in \Gamma_D, \quad (12.35)$$

$$\nabla u \cdot n = g_N, \quad x \in \Gamma_N, \quad (12.36)$$

with $\Gamma = \Gamma_D \cup \Gamma_N$. We obtain the variational formulation by multiplying with a test function $v \in V_0$, with

$$V_w = \{v \in H^1(\Omega) : v(x) = w(x), x \in \Gamma_D\}, \quad (12.37)$$

and integration over Ω . Using Green's theorem, we get the variational formulation: find $u \in V_{g_D}$, such that,

$$(\nabla u, \nabla v) = (f, v) + (g_N, v)_{L^2(\Gamma_N)}. \quad (12.38)$$

for all $v \in V_0$.

The Dirichlet boundary condition is enforced through the trial space, and is referred to as an *essential boundary condition*, whereas the Neumann boundary condition is enforced through the variational form, referred to as a *natural boundary condition*.

Galerkin finite element method

To compute approximate solutions to the Poisson equation, we can formulate a Galerkin method based on the variational formulation of the equation, replacing the Sobolev space V with a finite dimensional space V_h , constructed by a set of basis functions $\{\phi_i\}_{i=1}^M$, over a mesh \mathcal{T}_h , defined as a collection of elements $\{K_i\}_{i=1}^N$ and nodes $\{N_i\}_{i=1}^M$.

For the Poisson equation with homogeneous Dirichlet boundary conditions, the Galerkin element method takes the form: Find $U \in V_h$, such that,

$$(\nabla U, \nabla v) = (f, v), \quad v \in V_h, \quad (12.39)$$

with $V_h \subset H_0^1(\Omega)$.

The variational form (12.39) corresponds to a linear system of equations $Ax = b$, with $a_{ij} = (\phi_j, \phi_i)$, $x_j = U(N_j)$, and $b_i = (f, \phi_i)$, with $\phi_i(x)$ the basis function associated with the node N_i .

For V_h a piecewise polynomial space, we refer to (12.39) as a *Galerkin finite element method*.

12.4 Linear partial differential equations

The abstract problem

We can express a general linear partial differential equation as the abstract problem,

$$A(u) = f, \quad x \in \Omega, \quad (12.40)$$

with boundary conditions,

$$B(u) = g, \quad x \in \Gamma. \quad (12.41)$$

For a Hilbert space V , we can derive the variational formulation: find $u \in V$ such that,

$$a(u, v) = L(v), \quad v \in V, \quad (12.42)$$

with $a : V \times V \rightarrow \mathbb{R}$ a *bilinear form*, that is a function which is linear in both arguments, and $L : V \rightarrow \mathbb{R}$ a *linear form*, or *linear functional*, which is a linear function onto the scalar field \mathbb{R} .

Theorem 18 (Riesz representation theorem). *For every linear functional $L : V \rightarrow \mathbb{R}$ on the Hilbert space V , with inner product (\cdot, \cdot) , there exists a unique element $u \in V$, such that*

$$L(v) = (u, v), \quad \forall v \in V. \quad (12.43)$$

Existence and uniqueness

We can prove the existence of unique solutions to the variational problem (12.42), under certain conditions. Assume the bilinear form $a(\cdot, \cdot)$ is *symmetric*,

$$a(v, w) = a(w, v), \quad \forall v, w \in V, \quad (12.44)$$

and *coercive*, or *V-elliptic*,

$$a(v, v) \geq c_0 \|v\|_V, \quad v \in V, \quad (12.45)$$

with $c_0 > 0$, and $\|\cdot\|_V$ the norm on V . A symmetric and elliptic bilinear form defines an inner product on V , which induces a norm which we refer to as the *energy norm*,

$$\|w\|_E = a(w, w)^{1/2}. \quad (12.46)$$

But if the bilinear form is an inner product on V , by Riesz representation theorem there exists a unique $u \in V$, such that

$$a(u, v) = L(v). \quad (12.47)$$

If the bilinear form is not symmetric, we still have unique solution to (12.42) by the *Lax-Milgram theorem*, if the bilinear form is elliptic (12.45), and continuous,

$$a(u, v) \leq C_1 \|u\|_V \|v\|_V, \quad C_1 > 0, \quad (12.48)$$

with also the linear form continuous,

$$L(v) \leq C_2 \|v\|_V, \quad C_2 > 0. \quad (12.49)$$

Galerkin's method

In a Galerkin method we seek an approximation $U \in V_h$ such that

$$a(U, v) = L(v), \quad v \in V_h, \quad (12.50)$$

with $V_h \subset V$ a finite dimensional subspace, which in the case of a finite element method is a piecewise polynomial space.

The Galerkin approximation is optimal in the energy norm, since by Galerkin orthogonality,

$$a(u - U, v) = 0, \quad v \in V_h, \quad (12.51)$$

we have that

$$\begin{aligned} \|u - U\|_E^2 &= a(u - U, u - u_h) = a(u - U, u - v) + a(u - U, v - u_h) \\ &= a(u - U, u - v) \leq \|u - U\|_E \|u - v\|_E, \end{aligned}$$

so that

$$\|u - U\|_E \leq \|u - v\|_E, \quad v \in V_h. \quad (12.52)$$

12.5 Exercises

Problem 34. *Derive the variational formulation (12.38), and formulate the finite element method.*

Chapter 13

The heat equation

13.1 The heat equation

We consider the heat equation,

$$\dot{u}(x, t) - \Delta u(x, t) = f(x, t), \quad (x, t) \in \Omega \times I, \quad (13.1)$$

$$u(x, t) = 0, \quad (x, t) \in \Gamma \times I, \quad (13.2)$$

$$u(x, 0) = u_0(x), \quad x \in \Omega \quad (13.3)$$

on the domain $\Omega \subset \mathbb{R}^n$ with boundary Γ , and with the time interval $I = (0, T)$. To find an approximate solution to the heat equation, we use semi-discretization where space and time are discretized separately, using the finite element method and time stepping, respectively.

For each $t \in T$, multiply the equation by a test function $v \in V = H_0^1(\Omega)$ and integrate in space over Ω to get the variational formulation,

$$\int_{\Omega} \dot{u}(x, t) v(x) dx + \int_{\Omega} \nabla u(x, t) \cdot \nabla v(x) dx = \int_{\Omega} f(x, t) v(x) dx,$$

from which we formulate a finite element method: find $U \in V_h \subset V$, such that,

$$\int_{\Omega} \dot{U}(x, t) v(x) dx + \int_{\Omega} \nabla U(x, t) \cdot \nabla v(x) dx = \int_{\Omega} f(x, t) v(x) dx,$$

for all $v \in V_h$. The finite element method corresponds to the system of initial value problems,

$$M\dot{U}(t) + SU(t) = b(t), \quad (13.4)$$

with

$$m_{ij} = \int_{\Omega} \phi_j(x) \phi_i(x) dx, \quad (13.5)$$

$$s_{ij} = \int_{\Omega} \nabla \phi_j(x) \cdot \nabla \phi_i(x) dx, \quad (13.6)$$

$$b_i(t) = \int_{\Omega} f(x, t) \phi_i(x) dx, \quad (13.7)$$

which is solved by time stepping to get,

$$U(x, t) = \sum_{j=1}^M U_j(t) \phi_j(x). \quad (13.8)$$

13.2 Exercises

Problem 35. *Derive (13.4) from the variational formulation of the heat equation.*

Problem 36. *Multiply (13.1) by $u(x, t)$ and integrate over Ω , to show that for $f(x, t) = 0$,*

$$\frac{d}{dt} \|u(t)\|^2 \leq 0. \quad (13.9)$$