Numerical methods for PDEs

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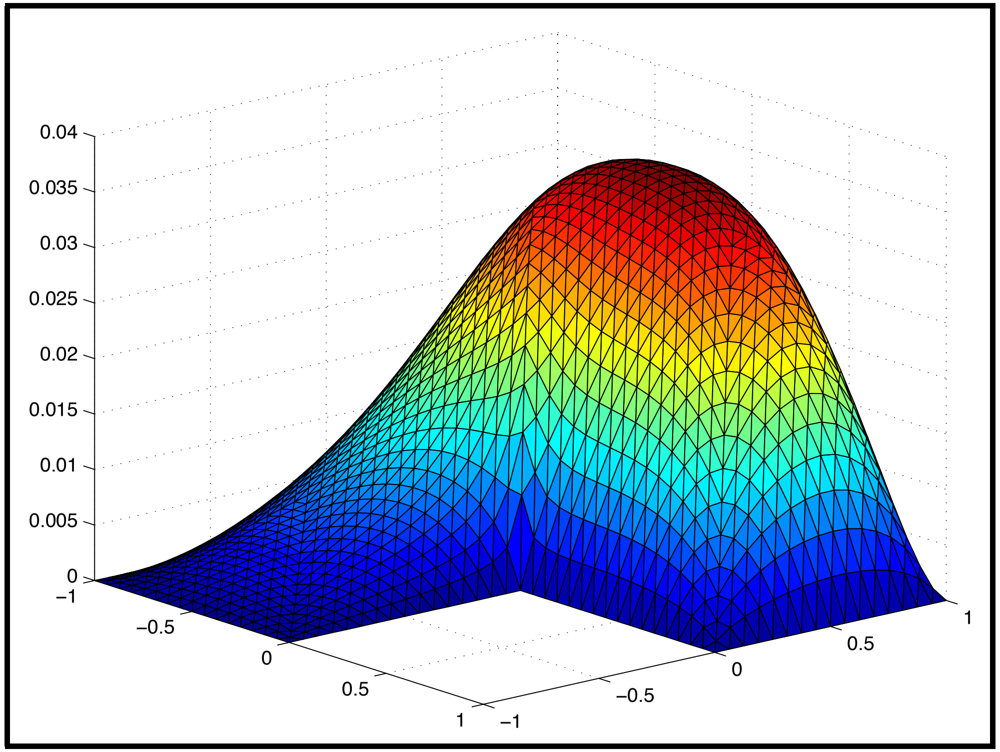

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Overview

- Motivation and background
- Elliptic boundary value problems
- Variational formulation
- Finite element spaces
- Implementational issues
- Parabolic initial boundary value problems

Introduction

Boundary value problem. Given a partial differential operator $\mathcal{L}$, a domain $\Omega \subset \mathbb{R}^d$, a boundary differential operator $\mathcal{B}$, boundary values g, and a source term f, seek a function $u : \Omega \to \mathbb{R}^q$ such that

$$\mathcal{L}(u) = f \text{ in } \Omega, \quad \mathcal{B}(u) = g \text{ on a part of the boundary } \partial\Omega.$$

Three main categories of boundary value problems (BVPs) for partial differential equations (PDEs):

- Elliptic BVPs
- Parabolic initial boundary value problems (IBVPs)
- Hyperbolic IBVPs, among them wave propagation problems and conservation laws

Rigorous mathematical definition $\longleftrightarrow$ Physics behind PDE-based models

What are "second-order scalar elliptic boundary value problems"?

- second-order: PDE features second-order spatial derivatives
- scalar: unknown is a function $u : \Omega \to \mathbb{R}$
- elliptic: "equilibrium character" (see following sections)

Example: stationary heat conduction

Fourier's law. Heat flow from hot to cold regions is linearly proportional to the gradient of the temperature:

$$\mathbf{j}(\mathbf{x}) = -\sigma(\mathbf{x})\nabla u(\mathbf{x}), \quad \mathbf{x} \in \Omega.$$

quantity	meaning	unit
$\mathbf{j}$	heat flux	$[\mathbf{j}] = 1\text{W}/\text{m}^2$
u	temperature	$[u] = 1\text{K}$
σ	heat conductivity	$[\sigma] = 1\text{W}/\text{m}$

- $\sigma = \sigma(\mathbf{x})$ for non-homogeneous materials (spatially varying heat conductivity)
- σ can even be discontinuous for composite materials
- from thermodynamic principles: $\sigma(\mathbf{x})$ is uniformly positive, i.e.

$$0 < \underline{\sigma} \leq \sigma(\mathbf{x}) \leq \overline{\sigma} < \infty \text{ for all } \mathbf{x} \in \Omega$$

- in the case of anisotropic materials: $\sigma(\mathbf{x})$ is a tensor, i.e.

$$\sigma(\mathbf{x}) \in \mathbb{R}^{d\times d}, \quad \sigma(\mathbf{x}) = \sigma(\mathbf{x})^\top, \quad 0 < \underline{\sigma}\|\boldsymbol{\xi}\|^2 \leq \boldsymbol{\xi}^\top \sigma(\mathbf{x})\boldsymbol{\xi} \leq \overline{\sigma}\|\boldsymbol{\xi}\|^2 < \infty, \quad \mathbf{x} \in \Omega$$

Example: stationary heat conduction

Conservation of energy. For all control volumes $V \subset \Omega$, it holds

$$\int_{\partial V} \mathbf{j} \cdot \mathbf{n} \, \mathrm{d}s = \int_V f \, \mathrm{d}\mathbf{x},$$

where f is the heat source or sink (unit $[f] = \mathrm{W}$, $f = f(\mathbf{x})$ can be discontinuous).

- By Gauss' theorem, we get the local form of energy conservation: $\boxed{\operatorname{div} \mathbf{j} = f \text{ in } \Omega}$
- Fourier's law & conservation of energy yields the PDE: $\boxed{-\operatorname{div}(\sigma \nabla u) = f \text{ in } \Omega}$
- If $\sigma \equiv const$, then it follows by rescaling the Poisson equation: $\boxed{-\Delta u = f \text{ in } \Omega}$

  Here, $\Delta = \dfrac{\partial^2}{\partial x_1^2} + \cdots \dfrac{\partial^2}{\partial x_d^2}$ is the Laplace operator.

Boundary conditions

- Dirichlet boundary condition: temperature u is fixed at the boundary

$$u = g \text{ on } \partial\Omega$$

- Neumann boundary condition: heat flux $\mathbf{j} = -\sigma\nabla u$ through $\partial\Omega$ is fixed

$$\sigma\frac{\partial u}{\partial \mathbf{n}} = h \text{ on } \partial\Omega$$

- Robin boundary condition: heat flux $\mathbf{j} = -\sigma\nabla u$ through $\partial\Omega$ depends linearly on u

$$-\sigma\frac{\partial u}{\partial \mathbf{n}} = q(u - u_0) \text{ on } \partial\Omega$$

$\rightsquigarrow$ convective cooling

Here, it holds that

$$0 < \underline{q} \leq q(\mathbf{x}) \leq \overline{q} < \infty \text{ for all } \mathbf{x} \in \partial\Omega$$

- Radiation condition: heat flux through $\partial\Omega$ depends nonlinearly on the local temperature

$$-\sigma\frac{\partial u}{\partial \mathbf{n}} = q|u - u_0|(u - u_0)^3 \text{ on } \partial\Omega$$

Characteristics of elliptic boundary value problems

- continuity: the temperature u must be continuous (jump in $u \Rightarrow \mathbf{j} = \infty$)
- normal component of $\mathbf{j}$ across a surfaces inside Ω must be continuous (jump in $\mathbf{j} \cdot \mathbf{n} \Rightarrow$ heat source f of infinite intensity)
- interior smoothness: u is smooth where f and σ are smooth
- non-locality: local alterations in f, g, h affect u everywhere in Ω
- quasi-locality: if local changes in f, g, h are confined to $V \subset \Omega$, then their effects decay away from V
- maximum principle: if $f(\mathbf{x}) \equiv 0$ for all $\mathbf{x} \in \Omega$, then

$$\inf_{\mathbf{z} \in \partial\Omega} u(\mathbf{z}) \leq u(\mathbf{x}) \leq \sup_{\mathbf{z} \in \partial\Omega} u(\mathbf{z}) \text{ for all } \mathbf{x} \in \Omega$$

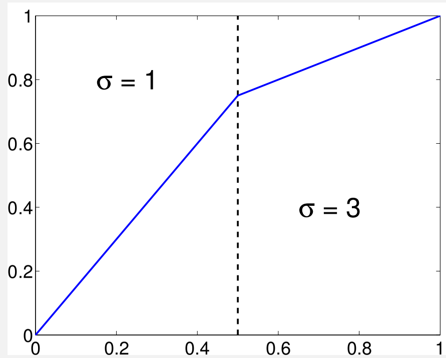
typical features of solutions of elliptic boundary value problems

Weak derivative

Example. One-dimensional stationary heat conduction model:

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\sigma\frac{\mathrm{d}}{\mathrm{d}x}u\right) = 0 \text{ in } (0,1), \quad u(0)=0, \quad u(1)=1, \quad \text{where } \sigma(x) = \begin{cases} 1, & 0<x<\frac{1}{2} \\ 3, & \frac{1}{2}<x<1 \end{cases}$$

Solution: $u(x) = \begin{cases} \frac{3}{2}x, & 0<x<\frac{1}{2} \\ \frac{1}{2}x+\frac{1}{2}, & \frac{1}{2}<x<1 \end{cases}$



For discontinuous σ, the (normal) continuity of $\mathbf{j}$ rules out the continuous differentiability of u.

How to make sense of $\frac{\mathrm{d}u}{\mathrm{d}x}$? $\rightsquigarrow$ weak derivative (piecewise derivative almost everywhere)

Definition. The weak partial derivative $\frac{\partial u}{\partial x_j}$, $j=1,\ldots,d$, of a locally integrable function $u:\Omega\to\mathbb{R}$ is, if it exists, a locally integrable function $\partial_{x_j}u:\Omega\to\mathbb{R}$ which satisfies

$$\int_\Omega \partial_{x_j}u v\,\mathrm{d}\mathbf{x} = -\int_\Omega u\frac{\partial v}{\partial x_j}\mathrm{d}\mathbf{x} \text{ for all } v\in C_0^\infty(\Omega),$$

where $C_0^\infty(\Omega)$ is the space of all compactly supported, smooth functions $\Omega\to\mathbb{R}$.

Variational formulation for Dirichlet problems

- Dirichlet problem:

$$\boxed{-\operatorname{div}(\sigma\nabla u) = f \text{ in } \Omega, \quad u = g \text{ on } \partial\Omega}$$

- Test the PDE with a smooth function $v \in C_0^\infty(\Omega)$ and integrate over the domain:

$$-\int_\Omega \operatorname{div}(\sigma\nabla u)v\,\mathrm{d}\mathbf{x} = \int_\Omega fv\,\mathrm{d}\mathbf{x}$$

- Apply integration by parts: Due to

$$\underbrace{\int_{\partial\Omega} \sigma\frac{\partial u}{\partial \mathbf{n}}v\,\mathrm{d}s}_{=0 \text{ because } v|_{\partial\Omega}=0} = \int_\Omega \operatorname{div}(\sigma\nabla uv)\,\mathrm{d}\mathbf{x} = \int_\Omega \sigma\nabla u\nabla v\,\mathrm{d}\mathbf{x} + \int_\Omega \operatorname{div}(\sigma\nabla u)v\,\mathrm{d}\mathbf{x},$$

it follows the variational formulation:

$$\boxed{\text{seek } u:\Omega\to\mathbb{R} \text{ with } u|_{\partial\Omega} = g \text{ such that } \int_\Omega \sigma\nabla u\nabla v\,\mathrm{d}\mathbf{x} = \int_\Omega fv\,\mathrm{d}\mathbf{x} \text{ for all } v \in C_0^\infty(\Omega)}$$

Variational formulation for general radiation condition

- Boundary value problem with general radiation condition:

$$-\operatorname{div}(\sigma\nabla u) = f \text{ in } \Omega, \quad -\sigma\frac{\partial u}{\partial \mathbf{n}} = \Psi(u) \text{ on } \partial\Omega$$

$$\text{where } \Psi(u) = \begin{cases} -h, & \text{Neumann problem} \\ q(u-u_0), & \text{Robin problem} \\ q|u-u_0|(u-u_0)^3, & \text{radiation problem} \end{cases}$$

- Test the PDE with a smooth function $v \in C^\infty(\overline{\Omega})$ and integrate over the domain:

$$-\int_\Omega \operatorname{div}(\sigma\nabla u)v\,\mathrm{d}\mathbf{x} = \int_\Omega \sigma\nabla u\nabla v\,\mathrm{d}\mathbf{x} - \int_{\partial\Omega} \underbrace{\sigma\frac{\partial u}{\partial \mathbf{n}}}_{=-\Psi(u)} v\,\mathrm{d}s = \int_\Omega f v\,\mathrm{d}\mathbf{x}.$$

  This leads to the variational formulation:

$$\text{seek } u:\Omega\to\mathbb{R} \text{ such that } \int_\Omega \sigma\nabla u\nabla v\,\mathrm{d}\mathbf{x} + \int_{\partial\Omega}\Psi(u)v\,\mathrm{d}s = \int_\Omega f v\,\mathrm{d}\mathbf{x} \text{ for all } v\in C^\infty(\overline{\Omega})$$

- Variational formulation of the Neumann problem is recovered for $\Psi(u) = -h$.
  For $v \equiv 1$, it follows the compatibility condition

$$\int_{\partial\Omega} h\,\mathrm{d}s + \int_\Omega f\,\mathrm{d}\mathbf{x} = 0.$$

Functional analytical framework

Except for the radiation condition, we obtain a problem of the form

$$\boxed{\text{seek } u \in V \text{ such that } a(u,v) = \ell(v) \text{ for all } v \in V}$$

where V is a vector space of functions $\Omega \to \mathbb{R}$

$a(\cdot,\cdot)$ is a symmetric bilinear form $a : V \times V \to \mathbb{R}$

$\ell(\cdot)$ is a linear form $\ell : V \to \mathbb{R}$

Definition. Given an $\mathbb{R}$-vector space V, a linear form $\ell(\cdot)$ is a mapping $\ell : V \to \mathbb{R}$ that satisfies

$$\ell(\alpha u + \beta v) = \alpha \ell(u) + \beta \ell(v) \text{ for all } \alpha, \beta \in \mathbb{R} \text{ and } u, v \in V.$$

A bilinear form $a(\cdot,\cdot)$ on V is a mapping $a : V \times V \to \mathbb{R}$, which is linear in both arguments.

Definition. A bilinear form a on a $\mathbb{R}$-vector space V is called an inner product, if it is symmetric and positive definite, that is,

$$a(u,v) = a(v,u) \text{ for all } u,v \in V \quad \text{and} \quad a(u,u) > 0 \text{ for all } 0 \neq u \in V.$$

An inner product always defines a norm via

$$\|u\|_V = \sqrt{a(u,u)} \text{ for all } u \in V.$$

An $\mathbb{R}$-Hilbert space V is a complete vector space with inner product.

Functional analytical framework

Definition. A linear form $\ell : V \to \mathbb{R}$ on a Hilbert space V is continuous, if there exists a constant $C_\ell > 0$ such that

$$|\ell(v)| \leq C_\ell \|v\|_V \text{ for all } v \in V.$$

A bilinear form $a : V \times V \to \mathbb{R}$ on a Hilbert space V is continuous, if there exists a constant $C_a > 0$ such that

$$|a(u,v)| \leq C_a \|u\|_V \|v\|_V \text{ for all } u,v \in V.$$

The bilinear form $a : V \times V \to \mathbb{R}$ on a Hilbert space V is elliptic, if there exists a constant $c_a > 0$ such that

$$c_a \|u\|_V^2 \leq a(u,u) \text{ for all } u,v \in V.$$

Functional analytical framework

Lax-Milgram theorem. Assume that $a(\cdot,\cdot)$ is an elliptic, continuous bilinear form with ellipticity constant $c_a > 0$ on the Hilbert space V and assume that $\ell(\cdot)$ is a continuous linear form. Then, the linear variational problem

$$\text{seek } u \in V \text{ such that } a(u,v) = \ell(v) \text{ for all } v \in V \tag{1}$$

has a unique solution $u \in V$ that satisfies the stability estimate

$$\|u\|_V \leq \frac{1}{c_a} \sup_{0\neq v\in V} \frac{|\ell(v)|}{\|v\|_V}.$$

Proof. 1. Uniqueness of solutions: if both $u_1, u_2 \in V$ solve (1), then

$$a(u_1 - u_2, v) = 0 \text{ for all } v \in V \Rightarrow \|u_1 - u_2\|_V^2 \leq \frac{1}{c_a} a(u_1 - u_2, u_1 - u_2) = 0 \Rightarrow u_1 = u_2$$

2. Existence of solutions $\rightsquigarrow$ profound functional analysis (requires completeness of V)

3. Stability of solutions:

$$c_a \|u\|_V^2 \leq a(u,u) = \ell(u) \leq \sup_{0\neq v\in V} \frac{|\ell(v)|}{\|v\|_V} \|u\|_V$$

Functional analytical setting for Dirichlet problems

Question. What is V for the variational formulation

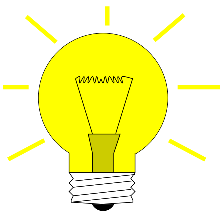
$$\text{seek } u : \Omega \to \mathbb{R} \text{ with } u|_{\partial\Omega} = 0 \text{ such that } \int_\Omega \sigma \nabla u \nabla v \,\mathrm{d}\mathbf{x} = \int_\Omega f v \,\mathrm{d}\mathbf{x} \text{ for all } v \in C_0^\infty(\Omega)?$$

- $a(u,v) = \int_\Omega \sigma \nabla u \nabla v \,\mathrm{d}\mathbf{x}$ is a symmetric bilinear form on $C_0^\infty(\Omega)$
- Is $a(\cdot,\cdot)$ positive definite?

$$\underline{\sigma} \|\nabla u\|_0^2 \le a(u,u) \text{ for all } u \in C_0^\infty(\Omega), \text{ where } \|u\|_0 := \sqrt{\int_\Omega u^2 \,\mathrm{d}\mathbf{x}} \text{ is the } L^2\text{-norm}$$

First Poincaré-Friedrichs inequality. It holds

$$\|u\|_0 \le \mathrm{diam}(\Omega) \|\nabla u\|_0 \text{ for all } u \in C_0^\infty(\Omega).$$



Idea. use $a(\cdot,\cdot)$ as an inner product on $C_0^\infty(\Omega)$: $\|u\|_V := \sqrt{a(u,u)}$

continuity / V-ellipticity of $a(\cdot,\cdot)$ trivially satisfied, since

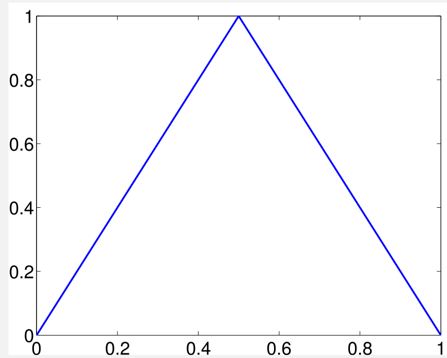
$$\|u\|_V^2 = a(u,u), \quad a(u,v) \le \|u\|_V \|v\|_V \quad \text{for all } u,v \in V$$

$\rightsquigarrow$ energy norm

Functional analytical setting for Dirichlet problems

Example. For $\Omega = (0,1)$, $\sigma \equiv 1$, and

$$u(x) = \begin{cases} 2x, & 0 < x < \frac{1}{2} \\ 2(1-x), & \frac{1}{2} < x < 1 \end{cases}$$

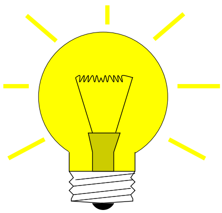


there holds

$$a(u,u) = \int_0^1 |u'(x)|^2 \,\mathrm{d}x = 4 < \infty$$

but $u \notin C_0^\infty(\Omega)$.

$\rightsquigarrow$ $C_0^\infty(\Omega)$ is not complete with respect to the energy norm



Idea. use trick from functional analysis

normed vector space $\xrightarrow{\text{completion}}$ complete vector space

$\rightsquigarrow$ set $V := \{v : \Omega \to \mathbb{R} \text{ with } v|_{\partial\Omega=0} : \|v\|_V < \infty\}$

Remark. V coincides the Sobolev space $H_0^1(\Omega)$ of all functions $v : \Omega \to \mathbb{R}$ with $v|_{\partial\Omega} = 0$ and finite norm

$$\|v\|_1 := \sqrt{\|v\|_0^2 + \|\nabla v\|_0^2} < \infty.$$

Functional analytical setting for Neumann problems

Question. What is V for the variational formulation

$$\text{seek } u:\Omega\to\mathbb{R} \text{ such that } \int_\Omega \sigma\nabla u\nabla v\,\mathrm{d}\mathbf{x} = \int_\Gamma hv\,\mathrm{d}s + \int_\Omega fv\,\mathrm{d}\mathbf{x} \text{ for all } v\in C^\infty(\overline{\Omega})$$

- same bilinear form as for the Dirichlet problem but different space!
- Obvious: $a(u,u)=0$ if $u\equiv const$ on Ω $\rightsquigarrow$ $a(\cdot,\cdot)$ is no inner product on $C^\infty(\overline{\Omega})$

Second Poincaré-Friedrichs inequality. If Ω is a bounded domain, then there is a constant c_{PF} such that

$$\|u\|_0 \le c_{PF}\|\nabla u\|_0 \text{ for all } u\in C_\star^\infty(\overline{\Omega}) := \left\{v\in C^\infty(\overline{\Omega}) : \int_\Omega v\,\mathrm{d}\mathbf{x}=0\right\}.$$

- $a(\cdot,\cdot)$ is an inner product on $C_\star^\infty(\overline{\Omega})$
- appropriate energy space is

$$V := \left\{v:\Omega\to\mathbb{R} \text{ with } \int_\Omega v\,\mathrm{d}\mathbf{x}=0 : \|v\|_V<\infty\right\}$$

Remark. V coincides the Sobolev space $H_\star^1(\Omega)$ of all functions $v:\Omega\to\mathbb{R}$ with vanishing mean and finite norm

$$\|v\|_1 := \sqrt{\|v\|_0^2+\|\nabla v\|_0^2}<\infty.$$

Essential and natural boundary conditions

Question. What happens in case of arbitrary Dirichlet boundary conditions $u|_{\partial\Omega} = g$?

- Let $\widetilde{g} : \Omega \to \mathbb{R}$ be an extension of g such that $\widetilde{g}|_{\partial\Omega} = g$
- variational formulation:

$$\text{seek } u \in \widetilde{g} + H_0^1(\Omega) \text{ such that } \int_\Omega \sigma \nabla u \nabla v \, d\mathbf{x} = \int_\Omega f v \, d\mathbf{x} \text{ for all } v \in H_0^1(\Omega)$$

- reformulation in order to match the Lax-Milgram lemma:

$$\text{seek } u_0 \in H_0^1(\Omega) \text{ such that } \int_\Omega \sigma \nabla u_0 \nabla v \, d\mathbf{x} = \int_\Omega f v \, d\mathbf{x} - \int_\Omega \sigma \nabla \widetilde{g} \nabla v \, d\mathbf{x} \text{ for all } v \in H_0^1(\Omega)$$

- the functional

$$\ell(v) := \int_\Omega f v \, d\mathbf{x} - \int_\Omega \sigma \nabla \widetilde{g} \nabla v \, d\mathbf{x}$$

  has to be continuous on $H_0^1(\Omega)$ $\quad \rightsquigarrow \widetilde{g} \in H^1(\Omega) := \{v : \Omega \to \mathbb{R} : \|v\|_1 < \infty\}$
- it holds

$$|\ell(v)| \leq \|f\|_0 \|v\|_0 + \overline{\sigma} \|\nabla \widetilde{g}\|_0 \|\nabla v\|_0 \leq C_\ell \|v\|_1$$

Dirichlet boundary conditions are directly imposed on the trial and test spaces ($\rightsquigarrow$ essential boundary conditions), whereas Neumann boundary conditions are automatically satisfied ($\rightsquigarrow$ natural boundary conditions).

Dirichlet principle

Consider the variational problem

$$\text{seek } u \in V \text{ such that } a(u,v) = \ell(v) \text{ for all } v \in V, \tag{2}$$

where $a(\cdot,\cdot)$ is a V-elliptic, continuous, and symmetric bilinear form and $\ell(\cdot)$ is a continuous linear form.

Theorem (Dirichlet principle). The solution of the variational problem (2) is the unique minimizer of the quadratic energy functional

$$J(v) = \frac{1}{2}a(v,v) - \ell(v).$$

Proof. Lax-Milgram lemma implies existence and uniqueness of the solution u to (2). Then, using $a(u,v) = \ell(v)$ for all $V \in v$, it holds

$$\begin{aligned} J(v) - J(u) &= \frac{1}{2}a(v,v) - \frac{1}{2}a(u,u) - \ell(v-u) = \frac{1}{2}a(v,v) - \frac{1}{2}a(u,u) - a(u,v-u) \\ &= \frac{1}{2}a(v-u,v-u) \geq c_a\|u-v\|_V^2. \end{aligned}$$

This implies $J(v) > J(u)$ for all $u \neq v \in V$. Conversely, u is the unique minimizer of $J(v)$.

Dirichlet principle

Result. The variational formulations of linear, scalar, second-order elliptic boundary value problems are equivalent to minimization problems for quadratic functionals (also known as Dirichlet forms or energy functionals).

Analogy. $\longrightarrow$ parabola

$$J(v) = \frac{1}{2}a(v,v) - \ell(v) \quad \Longleftrightarrow \quad f(x) = ax^2 + bx$$