Applied Analytical Methods, part I Basic Variational Structures and Methods

150950

E. van Groesen
Applied Analysis & Mathematical Physics
Faculty of Mathematical Sciences,
University of Twente

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Chapter 1

Introduction

In this course we consider problems with a variational structure and introduce specific methods to study these. The emphasis is on infinite-dimensional problems, since the origin of the problems lead to initial-boundary-value problems for partial or integral differential equations. Many results of finite dimensional case can and will be generalized.

Just as important as the introduction of the mathematical theory, is the second aim to illustrate where and how optimization/variational problems arise in nature and technical sciences, and how such a specific property can help to study and understand the problem[1].

Below we present a brief overview of the contents of the course.

1.1 General formulation of optimisation problems

Generally speaking, for an optimisation problem we have the following basic ingredients:

- a set of admissible elements $\mathcal{M}$, usually some subset of an (infinite dimensional) space $\mathcal{U}$;
- a functional $\mathcal{L}$, defined on $\mathcal{U}$ (or only on $\mathcal{M}$).

The optimisation problem of $\mathcal{L}$ on $\mathcal{M}$ concerns questions about an element $\hat{u}$ that minimizes the functional on the set of admissible elements, denoted by

$$\hat{u} \in \text{Min } \{\mathcal{L}(u) \mid u \in \mathcal{M} \},$$

which is by definition an element for which

$$\mathcal{L}(\hat{u}) \leq \mathcal{L}(u) \quad \text{for all} \quad u \in \mathcal{M}.$$

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[1] In other disciplines, economy, life-sciences, etc. optimisation problems are also abundant; we will restrict ourselves and mainly deal with applications form the natural and technical sciences.

These questions may deal with the existence, the uniqueness, and the characterization and computation of the minimizer.

We will mainly deal with the *characterisation* of the minimizer (and more general critical points); instead of proving 'existence' of minimisers. We will concentrate on the equation(s) that have to be satisfied by such a critical point; a local investigation near the point will show that for density functionals on function spaces, the element $\hat{u}$ usually satifies some (ordinary or partial) differential equation, the *Euler-Lagrange equation.*
The actual calculation of minimising elements can be done by using numerical methods.

1.2 Mathematical method of local investigation

In real analysis courses at an introductory level, functions of one or more variables are considered. The definition of differentiation of functions is a vital part of such courses, and a standard result is the following

> **Algorithm of Fermat**, for 1-D optimisation problems.
> If the differentiable scalar function of one variable $f : \mathcal{R} \to \mathcal{R}$ attains a (local) extreme value at the point $\hat{x}$, then the derivative at that point vanishes:
>
> $$f'(\hat{x}) = 0.$$

Viewed as a condition for a point to be an extremal element, this condition is necessary but not sufficient; every point, including saddle points, that satisfy this property are called stationary, or critical, points.

Knowing the above result for functions of one variable, the generalisation to functions of more variables, n-dimensional problems, is remarkably simple using partial derivatives to reduce the problem to n 1-D problems, as follows.
For $F : \mathcal{R}^n \to \mathcal{R}$, let ∇F be the gradient of the function, the column vector

$$\nabla F(x) = \begin{pmatrix} \partial_{x_1} F(x) \\ ... \\ \partial_{x_n} F(x) \end{pmatrix}.$$

Recall that the gradient is related to the (Frechet-) derivative using the standard innerproduct and is defined with the notion of directional derivative as follows: At the point x the directional derivative in the direction η is found by differentiating the scalar function obtained by restricting F to the line through x in the direction η, i.e. the function

$$\varepsilon \to F(x + \varepsilon\eta),$$

and so

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} F(x + \varepsilon\eta) \equiv DF(x)\eta \equiv \nabla F(x) \cdot \eta.$$

If x minimizes F on $\mathcal{R}^n$, this point certainly minimizes the restriction (for $\varepsilon = 0$), and hence the directional derivative vanishes in every direction η:

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} F(x + \varepsilon\eta) = 0.$$

From $\nabla F(x) \cdot \eta = 0$ for all η, it then follows that

$$\nabla F(x) = 0.$$

This is the direct generalisation of Fermat's algorithm to n-dimensional optimization problems.

When the space of definition for a scalar function is infinite dimensional (the function is then usually called a function*al*), the above can be generalised as follows:

- by restricting the functional to one dimensional lines the notion of directional derivative can be defined just as easily; it will be called the *first variation* in that case;
- when dealing with density-functionals, a generalisation of the gradient can be defined and will lead to the notion of *variational derivative.* The specific expression is related to the choice of the L_2 innerproduct for functions under consideration. *Lagrange's Lemma* is the result that enables the identification of the first variation with the variational derivative (modulo certain boundary conditions and some smoothness assumptions).

The typical notation to be used in the following for the variational derivative is $\delta\mathcal{L}(u)$, and Fermat's algorithm generalises to

$$\delta\mathcal{L}(u) = 0$$

as the condition for a minimizing element. This equation is most times a differential equation, replacing the algebraic equation $\nabla F(x) = 0$ that is obtained for a minimzer of a function of a finite number of variables.
Just as in finite dimensions, the second derivative may reflect minimisation properties, and in general provide insight into the character of a critical point. In the Calculus of Variations these aspect are dealt with in the *theory of first and second variation.*

1.3 Optimality in the natural sciences

> *"...... je suis convaincu que par tout la nature agit selon quelque principe d'un maximum ou minimum."* (Euler, 1746)

This quotation of one of the greatest scientists that shaped the modern mathematical description and investigation of the natural sciences, expresses clearly the underlying expectation. The belief that optimization was important to describe natural phenomena was verified by Euler for various problems, and exploited to present a more thorough investigation of the problems. More far reaching conclusions were drawn by some other scientists:

> *"...... des loix du mouvement ou l'action est toujours employee avec la plus grande economie, demontreront l'existence de l'Etre supreme ... "*, (Maupertuis, 1757)

but this point of view belongs to metaphysics, and is as such not very fruitful for a deeper investigation[2].

Actually, optimization problems are known already from ancient times; well known is *Dido's problem*: the problem to find the plain domain of largest area given the circumference of the domain. Many other problems can also be formulated as *geodetic problems*, where one investigates those curves (or surfaces) with the property that a functional measuring the length (or the area) is as small as possible. A major example is the following

> **Fermat's principle**, 1662
> The actual trajectory of a light ray between two points in an inhomogeneous medium has the property that the time (or optical length) required to transverse the curve is as small as possible when compared to the time required for any other curve between the points.

In fact, the investigation of this principle led Fermat to the mathematical result stated above as Fermat's algorithm[3].

From Fermat's principle, *Snell's law* can be derived about the breaking of light between two media. A dual point of view (looking for the evolution of light fronts, the surfaces that can be reached by the light from a point source in a give time) was investigated by Huygens, 1695. *Huygen's principle*, of vital importance for the basic understanding of light propagation, can be considered as a major example of what later has become known as duality methods.

These historical remarks make it clear that, although the analytical methods of the classical Calculus of Variations were developed in the eighteenth century by scientists like Newton, Euler and Lagrange, some basic ideas can already be found in the seventeenth century. From a more closer historical investigation

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[2] It should be noted, however, that modern theoretical physicists who look for "a theory of everything" (Grand Universal Theory) actually search for functionals (Lagrangians) that produce the desired unified field equations upon optimization, just as Einsteins general theory of relativity is based on a minimality principle.

[3] Fermat did not write down the actual equation; he reasoned that small variations near a minimizer produces a higher order variation in the function, the fundamental idea that leads to the result and justifies to adhere his name to the mathematical algorithm. Fermat didn't know the concept of derivative of functions other than polynomials; it was Leibniz who introduced in 1684 the concept of derivative of arbitrary functions.

it becomes clear that practical problems from physics provided the initial motivation for the beautiful mathematical theory that has been developed since then[4].

1.4 Dynamical systems with a variational structure

Except from problems that have by their very nature an “obvious” formulation as a minimization problem (minimum length, minimum costs, etc), there are many problems for which such an extremizing property exists, but not so obvious. Important examples can be found in dynamical systems.

The *principle of minimum (potential) energy* leads to equilibrium states for which the total energy is minimal (the kinetic energy vanishes for equilibria). For nontrivial dynamic evolutions in certain systems, a less intuitive quantity, the “action” (see the quotation of Maupertuis), turns out to be an important functional; actual evolutions correspond to saddle points (not extremizers in general) of this functional. Formulations of such systems were studied by Lagrange, Hamilton etc., and the many results are collected in what is now called *Classical Mechanics*, a well structured set of methods and results to study dynamical systems of collection of mass points, mechanical (rigid) structures etc. Nowadays, much effort is done to generalize these ideas to continuous systems, in particular to fluid dynamics, like water waves, and more general field theories. In this course we will deal with these modern aspects, particularly in Part II.

The systems referred to above, Lagrangian and Hamiltonian systems, are roughly speaking, conservative (the energy is conserved), and the dynamic motions have a variational nature. But even for systems that do not have such a structure, it is still possible that certain solutions have some extremizing property. This is true, for instance, for Poisson systems which are generalisations of Hamiltonian systems. When these systems are 'degenerate', no dynamic variational principle for the evolution can be found (in a simple way). However the equations do contain some variational struture (that may be be somewhat hidden), which makes it possible that special (but important)solutions can be characterised in a variational way. These solutions can be equilibrium (time independent) solutions, but can also be 'steady state solutions'. Often these are called *coherent structures* and are characteristic for such problems; examples are phenomena like 'travelling waves', 'solitons' and 'vortices'; owing to their variational nature, these can be found in a systematic way.

Even when the system is not conservative, but (mainly) dissipative, such as in gradient and thermodynamic systems, equilibrium solutions can be found by exploiting variational structures in the equations.

In all these cases that the special solutions can be characterised variationally, numerical algorithms can be used (or designed) to calculate the solutions approximately.

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[4] The interested reader may consult such references like Goldstein, and Newman vol. 2.

1.5 Contents of the Lecture Notes

The basic methods and variational structures in the sciences are described in Part I.
Specifically, Chapter 2 deals with the standard local methods of first and second variation for problems without constraints, and applications are given in Chapter 3.
In Chapter 4 variational problems with constraints will be considered, with applications in Chapter 5. Lagrange's multiplier rule will be generalised for the case that the set of admissible functions is the (intersection of) level sets of given other functionals (equality constraints).
All these matters will be discussed; of course, the infinite dimensional setting will lead to various aspects that make the theory more difficult then the finite dimensional case, but the main ideas are comparable.
In Chapter 6 we will consider eigenvalue-problems for symmetric differential operators (the infinite dimensional analog of symmetric matrices) and characterize the eigenfunctions in a variational way; among others things, Fourier theory including the completeness of the set of eigenfunctons, will be treated.
The linear eigenvalue problems are related to minimisation of convex (quadratic) functionals. In Chapter 7 we deal with various other convex problems; when the functionals are no longer quadratic, but still convex, various advanced methods are available.
Part II mainly concerns more advanced variational theory for dynamical systems. Poisson structures are introduced, and generalisations of methods from classical mechanics to partial differential equations are described; this is particularly useful for wave equations that appear in fluid dynamics and optics.
In one Annex, MAPLE-commands for calculating directional derivatives, linearization and variational derivatives are described. In another Annex, a bird eye's view on functional analytic aspects is given.

Chapter 2

Unconstrained variational problems

2.1 Density functionals and function spaces

We will mainly deal with functionals defined on (subsets of) linear function spaces. We start to define the general notation for the function spaces, and then consider the typical functionals that will be considered. Some simple definitions and properties for linear and quadratic functionals are summarized.

2.1.1 Characteristics of infinite dimensional spaces

This section is meant to show (recall) in a nutshell the essential difference between finite and infinite dimensional spaces. The latter are essentially more difficult since ususally more than one norm is involved. When thinking about Eucledian space $\mathcal{R}^n$, we do not only think of its elements as the n-vectors, but almost also immediately on the norm (length) of these vectors. In this space, actually every norm is equivalent to the Eucledian norm $||x||^2 = \sum_1^n x_k^2$, which is in fact an innerproduct norm:

$$||x||^2 = \langle x, x\rangle, \text{ with } \langle x, y\rangle = \sum_1^n x_k y_k.$$

In other words, ususally we immediately think of $\mathcal{R}^n$ as an *inner product space*. Moreover, this space is *complete*: every Cauchy sequence has a convergent subsequence; equivalently: every bounded sequence has a convergent subsequence, equivalently: bounded and closed subsets are compact. As a consequence, *Weierstrasz' theorem* holds: a continuous function on a compact set attains its maximum and minimum value at some points of the set.

$\mathcal{R}^n$ with the usual inner product is the prime example of what has later become known as a *Hilbert space*: a complete inner product space. Functional analysis studies (a.o.) infinite dimensional spaces with such properties, and generalizations to *Banach spaces* (complete normed spaces). In such spaces many of the finite dimensional properties still hold, provided concepts of continuity and compactness are taken with respect to the norm of the space.

In many applications when dealing with function spaces, it is not the case that one norm (or inner product) is the most natural one; in fact, often the space itself (the precise properties of its elements) has to be found (depending on the specific application), and so are the most suitable norms. Then it is usually the case that the norms that are involved are not equivalent: one is bounded by the other, but essentially not the other way around: the other can become unbounded on elements that are bounded in the first one.
We will illustrate these general remarks, as a kind of warning, to the simplest example; we use Fourier analysis to illuminate some matters.

Exercise 1 Consider the space of "sufficiently smooth" functions on a standard interval that vanish at the end points:

$$\mathcal{U} := \{u : [0, \pi] \to \mathcal{R} \mid u(0) = 0, u(\pi) = 0\}.$$

We restrict to L_2-functions, i.e. functions for which

$$||u||^2 := \int_0^\pi u^2(x)dx < \infty.$$

This is a norm, that can be defined with the standard inner product

$$\langle u, v\rangle := \int_0^\pi u(x)v(x)dx \equiv \int u(x)v(x).$$

1. Since for these boundary conditions the set $\{\sin kx\} \mid_{k\geq 1}$ is a complete set (in the norm above), we can write any function as a Fourier sinus series:

$$u = \sum_{k=1}^{\infty} u_k \sin kx.$$

Then, as is easily verified, since the Fourier modes are orthogonal,

$$\langle \sin kx, \sin jx\rangle = \pi/2\delta_{k,j},$$

Parseval's identity holds:

$$\langle u, v\rangle = \pi/2 \sum_{k=1}^{\infty} u_k v_k \quad \textit{and} \quad ||u||^2 = \pi/2 \sum_{k=1}^{\infty} u_k^2.$$

2. On functions for which it is finite, the following expression $|| \ ||_1$ defines a norm (and corresponding inner product), the so-called H_1-norm (the Sobolev space of order one, a Hilbert space upon completion)

$$||u||_1^2 := \int_0^\pi u_x^2(x)dx = \pi/2\sum_{k=1}^{\infty} k^2 u_k^2.$$

Note that $||u||_1 = ||u_x||$.

3. To investigate the relation between these two norms, consider the following minimization problem:

$$\inf\{\int_0^\pi u_x^2(x)dx \mid \int_0^\pi u^2(x)dx = 1, u \in \mathcal{U}\} \quad \textit{value} = 1, \quad \textit{attained for } u = \sin x.$$

From this follows the important property that for all functions in $\mathcal{U}$ the Poincaré - Friedrichs inequality holds:

$$||u|| \leq ||u||_1, \text{i.e.} \int_0^\pi u^2(x)dx \leq \int_0^\pi u_x^2(x)dx.$$

On the other hand, the maximization problem has no solution:

$$\sup\{\int_0^\pi u_x^2(x)dx \mid \int_0^\pi u^2(x)dx = 1, u \in \mathcal{U}\} = \infty.$$

This is a simple example of non-equivalent norms; it is said that the $|| \ ||_1$-norm is stronger than the $|| \ ||$-norm: a set bounded in $|| \ ||$ norm can be unbounded in $|| \ ||_1$-norm, while the reverse is not possible.

4. Interpret the results above also in the light of Weierstrasz theorem in infinite dimensional spaces:
Show that $\inf\{||u||^2 \mid ||u_x|| = 1, u(0) = u(\pi) = 0\} = 0$, but that "inf" is not attained for a continuous function.
What about $\sup\{||u||^2 \mid ||u_x|| = 1, u(0) = u(\pi) = 0\}$.?

5. Characteristic as the above may be, it is nevertheless common practice (and in many ways very useful) to "approximate" an infinite dimensional space with finite dimensional spaces of increasing dimension. For the example under consideration, this is just Fourier truncation. Consider

$$\mathcal{T}_N := \{\sum_{k=1}^{N} u_k \sin kx \mid (u_1, \ldots, u_N) \in \mathcal{R}^N\}.$$

Then, as expected

$$\inf\{\int_0^\pi u_x^2(x)dx \mid \int_0^\pi u^2(x)dx = 1, u \in \mathcal{T}_N\} = 1,$$

but now also

$$\begin{aligned} \sup\{\int_0^\pi u_x^2(x)dx \quad &| \quad \int_0^\pi u^2(x)dx = 1, u \in \mathcal{T}_N\} = N^2, \\ \text{attained for } u \quad &= \quad \sin Nx. \end{aligned}$$

This shows that in every finite dimensional truncation, the two norms are equivalent, but that in the limit $N \to \infty$ they are not equivalent.

Reassuring and warning: Despite the essential differences between finite and infinite dimensional spaces, many ideas that were developed over centuries for finite dimensional systems, can (and will) be generalized in the following to infinite dimensional systems. Keeping a sufficiently general and formal point of view, not many problems will arise. However, as soon as existence problems appear (existence of solutions of differential equations or of extremization problems), care should be taken in the correct formulation, and the results may require some thorough (functional analytic) investigation. For practical reasons we will not dwell too much on these last topics (which are studied extensively in modern-day “nonlinear functional analysis").

2.1.2 Notation, function spaces

Let $\Omega \subset \mathcal{R}^n$ be a bounded or unbounded domain; $x = (x_1, \dots, x_n) \in \Omega$ denote the independent variables. The boundary of Ω will be denoted by $\partial\Omega$ (it may be empty when the domain is unbounded).

On Ω we consider m-vector functions $u : \Omega \to \mathcal{R}^m$; $u = (u_1, \dots, u_m)$ are the dependent variables. In general the functions have to satisfy certain continuity or differentiability properties; the linear space will be denoted by $\mathcal{U}$.

If $m > 1$, the scalar-product of the functions at each point will be denoted in the standard way as the $\mathcal{R}^m$-innerproduct:

$$u \cdot v := \sum_{k=1}^m u_k v_k.$$

In most of the examples, we will deal with spaces $\mathcal{U}$ embedded in $L_2(\Omega)$; this means that each function $u \in \mathcal{U}$ is square integrable:

$$\int_\Omega |u|^2 dx < \infty$$

The standard L_2-innerproduct will be used repeatedly: for functions $u, v \in \mathcal{U}$

$$\langle u, v\rangle \equiv \int_\Omega u(x) \cdot v(x) dx.$$

We will employ various notations to denote partial derivatives (reflecting the various notations that are used in the literature):

- In a few general formulae that will be given for completeness, we employ multi-index notation: for $\alpha = (\alpha_1, \ldots, \alpha_n), \alpha_k \in N$

  $$|\alpha| = \sum_{k=1}^{n} \alpha_k, \quad \partial^\alpha = \partial_1^{\alpha_1} \partial_2^{\alpha_2} \ldots \partial_n^{\alpha_n}.$$

  In an analogous way will use D^α to denote the "total" partial derivatives when applicable.

- In most of the specific examples, the components of x are spatial or time coordinates; in those cases we write for example (t, x, y, z) for these coordinates, and $u_t, u_x, u_{xy}, \ldots$ for the partial derivatives.

- However, partial derivatives (and total derivatives when no confusion can arise) will mosttimes be denoted by ∂_t, ∂_x, etc..

In the following we will also use the standard operations for scalar functions φ and vector functions u on Ω:

$$\begin{array}{lllll}
\text{div } u & \equiv & \nabla \cdot u & = & \sum \partial_k u_k & \textit{divergence} \\
\text{grad } \phi & \equiv & \nabla \phi & = & (\partial_1 \phi, \ldots, \partial_n \phi) & \textit{gradient} \\
\text{rot } u & \equiv & \nabla \times u & = & & \textit{rotation(curl)} \\
\Delta \phi & \equiv & \text{div grad } \phi & = & \sum \partial_k^2 \phi & \textit{Laplaceoperator}
\end{array}$$

The space of *test functions* will play a dominant role in the following. This space will be denoted by $C_0^\infty(\Omega)$, and consists of infinitely often differentiable functions that have compact support in the interior of Ω.

Exercise 2 Show that when the interior of Ω is not empty, then $C_0^\infty(\Omega)$ is not empty; use the following facts.

1. Suppose that 0 is an interior point of Ω; then, for sufficietly small $\delta_0 > 0$, the ball with radius δ_0 belongs to Ω.

2. Show that the following two-paramter family of (scalar-) functions belong to $C_0^\infty(\Omega)$ for $0 < \delta < \delta_0, a \in R$:

   $$\phi_{a,\delta}(x) = \begin{cases} \exp\left[-\frac{a^2}{\delta^2 - |x|^2}\right] & \text{for} \quad |x| < \delta, \\ 0 & \text{for} \quad |x| \geq \delta \end{cases}$$

3. The family above consists of non-negative test functions; construct by differentiation test functions that are not sign definite, for instance functions with mean value zero.

2.1.3 Boundary conditions and constraints

The set $\mathcal{M}$ that will be the set on which the minimizing element of a given functional will be sought, is usually called the set of *admissible elements*; they are the elements allowed to participate in the comparison of the function values. This set will usually be a subset of a function space $\mathcal{U}$. Its elements will furthermore be specified by the fact that they satisfy certain boundary conditions or constraints. It will become clear in the following that these conditions are of a completely different type, and will be treated different accordingly. In fact, a proper treatment of boundary conditions is characteristic for the Calculus of Variations, and differs in this respect from the more general (abstract) optimization theory.

Boundary conditions are conditions on the restriction of the function and its derivatives to the boundary $\partial\Omega$. Typical examples are *Dirichlet boundary conditions*, where the function is prescribed at (part of) the boundary, and *Neumann boundary conditions* when (normal) derivatives are prescribed; we will see examples in the following.

Constraints (in the meaning that we will attach to this word in the following) are resrictions of the functions in the interior of the domain Ω. We will distinguish between *integral constraints*, for which some integrated expression is prescribed, and *point wise constraints* that restrict the functions in all, or certain, points of the domain.

To derive the governing equation for a minimizing element in the following section, an essential assumption will be that the test functions are admissible variations (in order to be able to apply Lagrange's Lemma). This means, roughly speaking, that constraints are excluded, and that boundary conditions (when present) are linear.
An important example for the following are sets $\mathcal{M}$ that are *affine spaces*, i.e. for which there exists a subspace $\mathcal{U}_0$ such that for each $\hat{u} \in \mathcal{M}$

$$\mathcal{M} = \{\hat{u}\} + \mathcal{U}_0.$$

The problem is unconstrained, and we talk about *unconstrained variational problems*, when moreover

$$C_0^\infty(\Omega) \subset \mathcal{U}_0.$$

In this chapter we will deal with such problems. The geometric picture is clear: $\mathcal{M}$ is a translation of the linear space $\mathcal{U}_0$, and for each point $\hat{u} \in \mathcal{M}$ it holds that the line in the direction η, for each test function η, belongs completely to the set of admissible elements:

$$\hat{u} + \varepsilon\eta \in \mathcal{M}, \text{ for all } \varepsilon \in \mathcal{R}, \text{ for each } \eta \in C_0^\infty(\Omega).$$

2.1.4 Tangent space to manifolds

Somewhat more general than in the previous subsection, consider the case that $\mathcal{M}$ is “smooth” manifold. Let $T_u\mathcal{M}$ denote the *tangent space* to $\mathcal{M}$ at the point u. By definition, the tangent space $T_u\mathcal{M}$ consists of all tangent vectors at u, i.e. of all the derivatives of curves on $\mathcal{M}$ through u (see Fig. 2.1):

$$\begin{aligned} v &\in T_u\mathcal{M} \text{ iff there exists a curve } \varphi : (-\varepsilon, \varepsilon) \subset \mathcal{R} \to \mathcal{M} \text{ such that} \\ \varphi(0) &= u \text{ and } \left.\frac{d}{d\varepsilon}\varphi(\varepsilon)\right|_{\varepsilon=0} = v. \end{aligned}$$

These tangent vectors define the linear space $T_u\mathcal{M}$. The afine space obtained by translating $T_u\mathcal{M}$ over u is the tangent plane to $\mathcal{M}$ at u; see Fig. 2.1

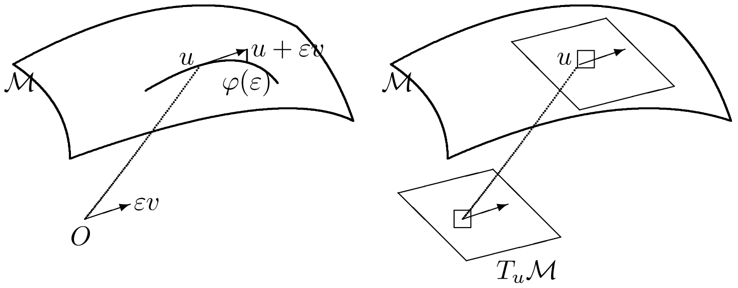

Figure 2.1: A tangent vector v to the manifold $\mathcal{M}$ at a point u defines a line that is tangent to a curve on $\mathcal{M}$,; the set of such tangent vectors defines the tangent space $T_u\mathcal{M}$ at u.

In the following we use the notation $T_u^*\mathcal{M}$ for the cotangent space, which is by definition the set of all linear functionals on the tangent space. For a given linear functional on $T_u\mathcal{M}$, say $\ell \in T_u^*\mathcal{M}$, and a tangent vector $v \in T_u\mathcal{M}$, the real number $\ell(v)$ is usually written like an inner product

$$\ell(v) = \langle \ell, v \rangle,$$

emphasizing that the pairing between tangent and cotangent space is a bilinear operation.

In the Calculus of Variations, elements v from the tangent space are usually called admissible variations: they are such that with u, the element $u + \varepsilon v$ belongs to $\mathcal{M}$ up to terms of order $\mathcal{O}(\varepsilon^2)$ for small real ε.

In the special case that $\mathcal{M}$ is an affine space as in the previous subsection, the tangent space is the translated linear space: for an affine space, it holds for all $u \in \mathcal{M}$

$$\mathcal{M} = \{u\} + T_u\mathcal{M}$$

and, actually, $T_u\mathcal{M}$ does not depend on u: $T_u\mathcal{M} = U_0$.

Exercise 3 For given functions $f \neq 0$ on Ω and ϕ on $\partial\Omega$, consider the three different sets of scalar functions u (smoothness is not specified):

$$\begin{aligned}
\mathcal{M}^1 &= \{u \mid u(x) = \phi(x) \ for\ x \in \partial\Omega\} \\
\mathcal{M}^2 &= \mathcal{M}^1 \cap \{u \mid \langle u, f\rangle = 2\} \\
\mathcal{M}^3 &= \{u \mid \langle u, u\rangle = 1\}
\end{aligned}$$

1. Show that both $\mathcal{M}^1$ and $\mathcal{M}^2$ are affine spaces, but that $\mathcal{M}^3$ is not affine.

2. Determine the tangent space at a certain point for each of the sets.

3. Show that

$$C_0^\infty \subset \mathcal{M}_0^1, \quad C_0^\infty \not\subset \mathcal{M}_0^2$$

where M_0^1, M_0^2 are the linear spaces connected to M^1, M^2.

With the more general notion of tangent space, we can make the definition of unconstrained problem more explicit.

Definition 4 *The variational problem for a functional on a domain of definition $\mathcal{M}$ is called an unconstrained variational problem if (at each $u \in \mathcal{M}$) the tangent space contains all test functions:*

$$C_0^\infty(\Omega) \subset T_u\mathcal{M}. \tag{2.1}$$

If that is not the case, it is called a constrained variational problem.

2.1.5 Density functionals

The density functionals that will be considered are typically of the following form

$$\mathcal{L}(u) = \int_\Omega L[u](x)dx.$$

Here, $L[u] \in R$ is an expression that depends on the point $x \in \Omega$, on $u(x)$ and on derivatives of u at the point x. Hence, given L as a function of its arguments, for a given point x and a sufficiently smooth function u, the value $L[u](x)$ can be calculated. The functions L is known as the *Lagrangian* (density) of the functional $\mathcal{L}$.
The *order of the Lagrangian* L is p if the highest derivative of u appearing in $L[u]$ is of the order p.

Assumption. In the following we assume mosttimes that the functionals are such that the order of the Lagrangian is finite[1], and that the Lagrangian, as a function of its arguments, is at least twice continuously differentiable.

Exercise 5 *Single integral functionals*
When the domain of definition of the functions is an interval ($m = 1$), the functionals are called single integral functionals.
In the classical example from mechanics, the time is the independent variable, $t \in [t_0, t_1] \equiv \Omega \subset R$, (generalized) coordinates $q = (q_1, \dots, q_N)$ are the dependent variables, and the simplest Lagrangian is of the form

$$L : \mathcal{R} \times \mathcal{R}^N \times \mathcal{R}^N \to \mathcal{R}, \quad L[q](t) = L(t, q(t), \dot{q}(t))$$

where $\dot{q}$ is the time derivative.
Higher order derivatives may arise in describing one-dimensional elastic media for instance.

1. For given potential energy $V : \mathcal{R} \times \mathcal{R}^N \to \mathcal{R}$, and M a symmetric, positive definite $N \times N$ mass-matrix, the following action functional has the difference of kinetic and potential energy as Lagrangian:

$$\mathcal{L}(q) = \int_{t_0}^{t_1} \{\frac{1}{2}\dot{q} \cdot M\dot{q} - V(t, q(t)\}dt$$

2. A simple (linear) model for the vertical deflection $u(x)$ of a one-dimensional elastic medium will be found from a functional of the form

$$\mathcal{L}(u) = \int_a^b \{\frac{1}{2}\mu(x)u_{xx}^2 + \frac{1}{2}\sigma(x)u_x^2 - f(x)u\}dx;$$

here μ and σ are certain material functions, and f an applied force.

Exercise 6 *Multiple integral functionals*

1. An elastic medium occupying a region $\Omega \subset \mathcal{R}^3$ is the 3-dimensional analog of the example above:

$$\mathcal{L}(u) = \int_\Omega \{\frac{1}{2}\mu(x)(\Delta u)^2 + \frac{1}{2}\sigma(x)|\nabla u|^2 - f(x)u\}dx;$$

2. The area of a surface in $\mathcal{R}^3$ that is described as the graph of a function by $(x, y, u(x, y))$ for $(x, y) \in \Omega \subset \mathcal{R}^2$ is given by

$$\int_\Omega \sqrt{1 + |\nabla u|^2} dxdy.$$

---

[1] A density depending only on the derivatives at the point under consideration is called a *local density*, to distinguish from a *non-local density* where it may also depend on u or its derivatives at another place. Occasionally we will meet integrals with a non-local density; these are mostly quadratic functionals of the form $\langle u, Ru\rangle$ where R is an integral operator or a more general pseudo-differential operator.

2.1.6 Boundary functionals

A boundary functional is by definition an integral over the boundary $\partial\Omega$ of an expression that contains the restriction of the function u defined on Ω and its derivatives (not necessarily derivatives along the boundary!):

$$\mathcal{L}_b(u) = \int_{\partial\Omega} b[u](x)dx$$

Exercise 7 *1.* For the single integral functional for elastica, a boundary functional is for example

$$\mathcal{L}_b(u) = u(a) - u_x(b).$$

For the 3-dimensional analog, an example is

$$\mathcal{L}_b(u) = \int_{\partial\Omega_1} \{u\phi(x)\}dx + \int_{\partial\Omega_2} \{\frac{\partial u}{\partial n}\psi(x)\}dx$$

where ϕ and ψ are given functions on the parts of the boundary $\partial\Omega_1$ and $\partial\Omega_2$; the notation $\frac{\partial u}{\partial n}$ denotes the normal derivative.

2. A density functional on a domain $\Omega \subset R^n$ of the form

$$\mathcal{L}_0(u) = \int_\Omega div\ P[u](x)dx$$

with P a given n-vector field that depends on x, u and derivatives of u, can be reduced to a boundary integral by using Gausz' theorem:

$$\mathcal{L}_0(u) = \int_{\partial\Omega} P[u](x) \cdot n$$

where n is the outward pointing normal to Ω.
Functionals of this type will be called *null-functionals* in the following.

2.1.7 Bilinear functionals and quadratic forms

Here we recall some general notions that will be used repeatedly in the following.

A functional ℓ defined on a linear space U is linear if for all $u, v \in U$ and all $\lambda \in \mathcal{R}$

$$\ell(u+v) = \ell(u) + \ell(v), \quad \ell(\lambda u) = \lambda\ell(u).$$

A functional $b : U \times U \to \mathcal{R}$ is a bilinear functional if it is linear in each of its arguments, so

$$\mathcal{U} \ni v \mapsto b(u, v) \text{ is linear for all } u \in \mathcal{U},$$

and

$$\mathcal{U} \ni u \mapsto b(u,v) \text{is linear for all } v \in \mathcal{U}.$$

A bilinear functional b can have special properties:

$$\begin{array}{rcl} symmetry & : & b(u,v) = b(v,u) \\ skew-symmetry & : & b(u,v) = -b(v,u) \\ non-degeneracy & : & \begin{cases} [b(u,v) = 0 \ \text{ for all } u] \Rightarrow v = 0 \\ [b(u,v) = 0 \ \text{ for all } v] \Rightarrow u = 0 \end{cases} \\ positive\ semi\ definiteness & : & b(u,u) \geq 0 \\ positive\ definiteness & : & b(u,u) > 0 \ \text{ for all } u \neq 0. \end{array}$$

Note the following fact:

$$b(u,u) = 0 \text{ if } b \text{ is skew-symmetric.}$$

A symmetric bilinear functional is a kind of generalized inner product; when it is positive definite, it is a true innerproduct. In all cases it defines a quadratic form.

Definition 8 *For given symmetric bilinear form b on U, the corresponding so-called quadratic form $a : U \to \mathcal{R}$ is defined by*

$$a(u) := b(u,u);$$

when a is positive definite, it is a norm, and b is an innerproduct; when a is positive semi definite, a is called a semi-norm.

Proposition 9 *For the symmetric bilinear functional b and the corresponding quadratic form a, the following relations hold:*

$$\begin{array}{rcl} a(u+v) & = & a(u) + 2b(u,v) + a(v), \\ b(u,v) & = & \frac{1}{4}[a(u+v) - a(u-v)], \\ a(u+v) + a(u-v) & = & 2[a(u) + a(v)]. \end{array}$$

When a is positive semi definite, Cauchy-Schwartz inequality holds:

$$|b(u,v)|^2 \leq a(u)a(v).$$

Exercise 10

1. Given a quadratic form, the symmetric bilinear functional can be found from $b(u,v) = \frac{1}{4}[a(u+v) - a(u-v)]$; hence there is a one to one relation between quadratic forms and symmetric bilinear functionals. Verify this.
2. Prove the Cauchy-Schwartz inequality for non-negative quadratic forms.

3. Under suitable conditions on the function σ, the following quadratic functional defines a norm; derive the corresponding bilinear functional, and write down the Cauchy Schwartz inequality:

$$a(u) = \int_a^b \{\sigma(x)u_x^2 + u^2\}dx.$$

4. The same for the more dimensional generalization

$$a(u) = \int_\Omega \{\sigma(x)|\nabla u|^2 + u^2\}dx.$$

2.2 Restriction of functionals

2.2.1 Example/Motivation.

Consider the one-parameter family of functions defined on the interval $[-1, 1]$

$$M = \{v|v(x) = a + x, a \in \mathcal{R}\}$$

where a is the parameter. When substituting in the functional

$$\mathcal{L}(u) = \int_{-1}^1 u^2 dx$$

there results $\mathcal{L}_M(v) = \int_{-1}^1 (a + x)^2 dx$ which can be calculated explicitly

$$L_M(v) = \int_{-1}^1 (a + x)^2 dx = 2a^2 + \frac{2}{3}$$

This means that on the one-parameter family of functions the functional reduces to an explicit function of the parameter. Stated differently: by restricting the domain of definition of the functional to a finite dimensional space (here the one-dimensional set of functions $v(x)$) the functional is restricted, and becomes a function in the parameters that define the finite dimensional subspace (here, the only parameter is a) .
The following exercises generalize this example.

2.2.2 Exercises

Exercise 11 Consider the functional

$$\mathcal{L}(u) = \int_{-1}^1 u^2 dx$$

The domain of definition of this functional is in principle the infinite dimensional set D :

$$D = \{u : [-1, 1] \to \mathcal{R}| \int_{-1}^1 u^2 dx < \infty\}$$

We will restrict the functional by taking various finite dimensional subspaces of D.

1. Let P_1 be the set of polynomials of degree at most one:

$$P_1 = \{a_0 + a_1 x | a_0, a_1\}$$

This is a two-dimensional set. Determine the restriction of the functional $\mathcal{L}$ to this set, i.e. determine the function $\mathcal{L}_{P_1}$ of two variables explicitly.

2. Construct the restriction of the functional on the sets of polynomials of higher degree, $P_{2,}P_3, P_4$ respectively.

3. Make a simple program in MAPLE to do these calculations.

Exercise 12 Consider the functional

$$\mathcal{L}(u) = \int_{-1}^{1} [u(x) - \sin(x)]^2 dx$$

Minimizing this functional is an example of the least square method to approximate the given function $\sin(x)$ by a function $u(x)$ from a given subset. Clearly, if any function $u(x)$ would be allowed, the solution of the minimization problem would be $u_{\min}(x) = \sin(x)$.

1. Restrict the functional to the sets $P_{2,}P_3$ respectively, and find the corresponding functions $\mathcal{L}_{P_2}, \mathcal{L}_{P_3}$.

2. Find the minimizers of these functions.

3. Write down the corresponding minimizing polynomials.

4. What is the relevance of these minimizing polynomials when looking for the minimizer of the functional $u_{\min}$? Interpret the minimizing polynomials as the projection of the function $\sin(x)$ on the set of polynomials.

5. To make the last even more explicit, show that a function u_P minimizes the given functional on a given set P :

$$u_P \in Min_{u \in P} \left\{ \int_{-1}^{1} [u(x) - \sin(x)]^2 dx \right\}$$

if and only if it is given by $u_P = \rho v_P$ with $\rho = \int_{-1}^{1} sin(x) v_P(x) dx$ where v is the solution of the maximization problem

$$v_P \in Max_{v \in P} \left\{ \int_{-1}^{1} v(x) \sin(x) dx \,|\, \int_{-1}^{1} v(x)^2 dx = 1 \right\}$$

6. Draw the corresponding situation for the projection of a given vector on a subspace, and show that the above is based on the identity (for L_2 -norm and - inner product)

$$||u - \sin||^2 = ||u||^2 - 2 < u, \sin > + || \sin ||^2$$

when substituting (like polar-coordinates)$u = \rho\, v$.

7. Find the projection of $\sin(x)$ (the least square approximation) on the polynomial sets for the norm $|| \; ||_1$ given by

$$||u||_1^2 = \int_{-1}^{1} u_x^2 dx$$

Exercise 13 Consider the functional

$$\mathcal{L}(u) = \int_{-1}^{1} [u_x^2 - \sin(x)u]dx$$

1. Restrict the functional to the sets P_2, P_3 respectively, and find the corresponding functions $\mathcal{L}_{P_2}, \mathcal{L}_{P_3}$.
2. What is the relevance of these minimizers when looking for the minimizer of the functional?

Exercise 14 Now consider the case that the domain of definition of the functional is further restricted to functions that vanish at the boundary points. For instance, then the polynomials of degree at most 3 is the set (verify)

$$P_3^0 = \{(b_0 + b_1 x)(1-x)(1+x)|b_0, b_1\}$$

Find now the minimiser of the previous functional $\mathcal{L}(u) = \int_{-1}^{1}[u_x^2 - \sin(x)u]dx$ on this set.

Exercise 15 *Maple*

1. Make a simple Maple program that restricts a given functional to a given finite dimensional space of parameterized functions, with as outcome the explicit restricted function of the parameters.
2. Verify that the program works correctly for the problems described above.

Exercise 16 *Multiple-integral functionals.*
Now consider functions $u(x, y)$ of two variables, defined on the square $\Omega = [-1, 1] \times [-1, 1]$.

1. Define the set P_2 of polynomials (of two variables) of degree at most 2, and determine the restriction to this set of the (so-called Dirichlet) functional

$$\mathcal{L}(u) = \int_{\Omega} |\nabla u|^2 dxdy \equiv \int_{\Omega} [u_x^2 + u_y^2] dxdy$$

2. Consider the following set of functions vanishing at the boundary

$$P^0 = \{p(x, y)(1-x)(1+x)(1-y)(1+y)|p \in P_2\}$$

Determine the projection (with the L_2 norm) of the function $u(x, y) = \cos(\pi x/2)\cos(\pi y/2)$ on the set P^0.

2.3 Theory of first variation: Euler - Lagrange equation

In this section we derive the generalization of Fermat's algorithm as announced in the introduction. It must be noted that this is in fact a local result: assuming the existence of a minimizer, we derive the anticipated result; no conditions are stated that guarantee the existence of a minimizer.

2.3.1 First variation and variational derivative

The aim is to consider the "derivative" of a functional. As stated already, it is natural to use the idea of directional derivative since then the problem is reduced to the differentiation of a scalar function of only one variable.
Hence, let u be a given function, and v an (arbitrary) variation. The classical notion "variation" refers to the fact that the original function u is embedded in a class of "varied" functions (a one-parameter family) of the form

$$\varepsilon \mapsto u + \varepsilon v.$$

Fixing v, this can be seen as a line in the function space going through the point u in the direction v. Restricting the functional to this line, it becomes a scalar function of one variable:

$$\varepsilon \mapsto \mathcal{L}(u + \varepsilon v).$$

The derivative of this function is then by definition the directional derivative, the first variation.

Definition 17 First variation
The first variation of a functional $\mathcal{L}$ *at* u *in the direction* v *is denoted by* $\delta\mathcal{L}(u;v)$ *and defined as*

$$\delta\mathcal{L}(u;v) = \left.\frac{d}{d\varepsilon}\mathcal{L}(u+\varepsilon v)\right|_{\varepsilon=0}. \tag{2.2}$$

In most cases, the first variation is linear in v (nonlinear in u in general). When it is linear in v (and continuous with respect to a topology on the space), it is also known as the Gateaux-derivative, the direct generalization of the directional derivative of a function on a finite dimensional space.

From the definition of first variation above, it follows directly that a linear approximation of $\mathcal{L}(u+\varepsilon v)$ is given as

$$\mathcal{L}(u+\varepsilon v) = \mathcal{L}(u) + \varepsilon\delta\mathcal{L}(u;v) + o(\varepsilon) \tag{2.3}$$

where, here and in the following, $o(\varepsilon)$ means terms that are of higher than first order in ε: $o(\varepsilon)/\varepsilon \mapsto 0$ for $\varepsilon \mapsto 0$.

The definition above applies to all kind of functionals. For density functionals that will occur most, it is usually possible to perform a partial integration and to rewrite $\delta\mathcal{L}(u;v)$ as the $L_2(\Omega)$-innerproduct of v and some function which will be denoted by[2] $\delta\mathcal{L}(u)$ (the direct generalization of the gradient of a function of a finite number of variables).
This may require the function u to be smooth enough, and usually a contribution consisting of an integration over the boundary appears in addition:

$$\delta\mathcal{L}(u;v) = \int_\Omega \delta\mathcal{L}(u)\cdot v + \int_{\partial\Omega} b(u;v) \tag{2.4}$$

If functions v are considered that vanish on the boundary, the boundary contribution vanishes identically. Therefore, we can use in particular the class of test functions $C_0^\infty(\Omega)$ to avoid these boundary contributions. Then we have the following notion.

Definition 18 *The function $\delta\mathcal{L}(u)$ on Ω defined by the condition*

$$\begin{aligned} \delta\mathcal{L}(u;\eta) &= <\delta\mathcal{L}(u),\eta> \\ &\equiv \int_\Omega \delta\mathcal{L}(u)\cdot\eta\, dx, \text{ for all } \eta\in C_0^\infty(\Omega) \end{aligned} \tag{2.5}$$

is called the variational derivative *of the functional $\mathcal{L}$ at the point u.*

It will follow from Lagrange's Lemma 23 below that when $\delta\mathcal{L}(u)$ is continuous, (2.5) indeed defines the function $\delta\mathcal{L}(u)$ uniquely. We will give various examples in the following to demonstrate the calculation of the variational derivative.

Remark 19 When we consider functionals on a manifold $\mathcal{M}$ in the following, and we want to stress the role of the function $\delta\mathcal{L}(u)$ in its relation to the linear functional $v\mapsto\delta\mathcal{L}(u;v)$, we will write $\delta\mathcal{L}(u)\in T_u^*\mathcal{M}$, where $T_u^*\mathcal{M}$ is the cotangent space. In this identification-process one has to remind that boundary-terms are disregarded. Instead of making the identification between the linear functionals $\delta\mathcal{L}(u;\cdot)$ and the variational derivative $\delta\mathcal{L}(u)$, it would be more correct to interpret $\delta\mathcal{L}(u)$ as a convenient notation for the linear functional $\delta\mathcal{L}(u;\cdot)$, and so to extend (2.5) to

$$\delta\mathcal{L}(u;v) = \langle\delta\mathcal{L}(u),v\rangle, \text{ for all } v\in T_u\mathcal{M} \tag{2.6}$$

with $\langle\ ,\ \rangle$ the duality map between $T_u\mathcal{M}$ and $T_u^*\mathcal{M}$. In the general formulae to follow we will use the notation (2.6); in the applications the formulae will be mostly exploited for the variational derivative, i.e. by taking for $\langle\ ,\ \rangle$ the L_2-innerproduct.

---

[2] For notational convenience we will exploit the notation $\delta\mathcal{L}(u)$, although in much of the literature the notation $\delta\mathcal{L}/\delta u$ is often used:

$$\delta\mathcal{L}(u)\equiv\frac{\delta\mathcal{L}}{\delta u}(u).$$

2.3.2 Stationarity condition

We now consider the basic optimization problem.
Let $\mathcal{M}$ be a smooth manifold, and, as before, let $T_u\mathcal{M}$ denote the tangent space to $\mathcal{M}$ at u. Recall that the elements v from the tangent space are the admissible variations: they are such that with u, the element $u + \varepsilon v$ belongs to $\mathcal{M}$ up to terms of order $\mathcal{O}(\varepsilon^2)$ for small real ε.

Considering $\mathcal{L}(u + \varepsilon v)$ for an admissible variation, in general this value will differ from $\mathcal{L}(u)$ in first order in ε as follows from (2.3). At critical points this difference is of higher (mosttimes second) order.

Definition 20 *A point $\hat{u}$ is called a* critical point, or stationary point*, of the functional $\mathcal{L}$ on the set $\mathcal{M}$ if the following holds:*

$$\delta\mathcal{L}(\hat{u}; v) = 0 \quad \textit{for all } v \in T_{\hat{u}}\mathcal{M}. \tag{2.7}$$

In the following we will occasionally use the notation $\hat{u} \in Crit\ \{\mathcal{L} \mid \mathcal{M}\ \}$

Of course, as in finite dimensions, local extrema, i.e. points at which $\mathcal{L}$ has an extreme value (maximal or minimal) when compared to neighbouring points in $\mathcal{M}$, are critical points.

Proposition 21 *If $\mathcal{L}$ has a local maximal or minimal value at $\bar{u}$, then $\bar{u}$ is a critical point of $\mathcal{L}$.*

This is a basic result in the theory of "first variation": *(2.7) gives the condition for a point to be a critical point, which is a necessary condition for a point to be a local maximum or minimum.*

2.3.3 Euler-Lagrange equation for unconstrained problems

It is possible to translate condition (2.7) into an explicit equation for $\hat{u}$ along the following lines.
Let $\hat{u}$ be a critical point of the unconstrained variational problem for $\mathcal{L}$ on $\mathcal{M}$. From the stationarity condition (2.7) and the fact that $T_u\mathcal{M} \supset C_0^\infty(\Omega)$, it follows that certainly it must hold that

$$\delta\mathcal{L}(\hat{u}; \eta) \equiv \langle \delta\mathcal{L}(\hat{u}), \eta \rangle = 0 \quad \text{for all } \eta \in C_0^\infty(\Omega). \tag{2.8}$$

This leads to the equation for $\hat{u}$.

Proposition 22 Euler-Lagrange equation
If $\hat{u}$ is a critical point of the unconstrained variational problem for $\mathcal{L}$ on M, then (provided $\delta\mathcal{L}(\hat{u})$ is a continuous function) $\hat{u}$ satisfies

$$\delta\mathcal{L}(\hat{u}) = 0. \tag{2.9}$$

This equation for $\hat{u}$ is called the Euler-Lagrange equation of the functional L.

The proof of this result is an immediate consequence of the first order condition (2.8) and the following basic Lemma.

Lemma 23 Lagrange's Lemma
Let f be a continuous function on Ω that is such that

$$\int_\Omega f(x)\eta(x)dx = 0 \textit{ for all } \eta \in C_0^\infty(\Omega).$$

Then f vanishes identically on (the interior of) Ω: $f(x) = 0$ for all $x \in \Omega$.

Exercise 24 *Prove Lagrange's Lemma.*

2.3.4 Natural boundary conditions

From the vanishing of the first variation for all test functions, the Euler-Lagrange equation is obtained. For unconstrained problems, the tangent space may contain more elements. Then, for a critical point it should also hold that the boundary contribution in (2.4) vanishes:

$$\int_{\partial\Omega} b(\hat{u}; v) = 0, \quad \text{for all} \quad v \in T_{\hat{u}}\mathcal{M}. \tag{2.10}$$

This condition may be satisfied automatically for $\hat{u} \in \mathcal{M}$, but it may also give certain conditions on $\hat{u}$ on the boundary $\partial\Omega$. In the latter case, these conditions are called natural boundary conditions: they appear as additional conditions for a critical point, not by the requirement that $\hat{u}$ should belong to $\mathcal{M}$, but from the stationarity condition (2.7) itself.

2.4 Theory of second variation

When for fixed v the function $\varepsilon \mapsto \mathcal{L}(u + \varepsilon v)$ is twice diferentiable, its second derivative leads to the following notion.

Definition 25 *The* second variation *of a functional $\mathcal{L}$ at u in the direction v is denoted by $\delta^2\mathcal{L}(u; v)$ and is defined as*

$$\delta^2\mathcal{L}(u; v) = \left.\frac{d^2}{d\varepsilon^2}\mathcal{L}(u + \varepsilon v)\right|_{\varepsilon=0}. \tag{2.11}$$

Hence we have

$$\mathcal{L}(u + \varepsilon v) = \mathcal{L}(u) + \varepsilon\delta\mathcal{L}(u; v) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{L}(u; v) + o(\varepsilon^2). \tag{2.12}$$

From this the following second order condition for an extremal element is obvious.

Proposition 26 *If $\hat{u}$ is a local extremal for $\mathcal{L}$, the second variation is sign-definite for all directions v in the tangent space.*
Specifically, if $\mathcal{L}$ has a (local) minimum at $\bar{u}$:

$$\mathcal{L}(\bar{u}) \leq \mathcal{L}(u) \textit{ for all } u \in \mathcal{M} \textit{ in a neighbourhood of } \bar{u}, \tag{2.13}$$

then

$$\delta^2\mathcal{L}(\bar{u}; v) \geq 0 \textit{ for all } v \in T_{\bar{u}}\mathcal{M}. \tag{2.14}$$

In most cases, the second variation $\delta^2\mathcal{L}(u; v)$ is quadratic in v. When it is, it can also be obtained as a repeated differentiation of the first variation. In fact, a bilinear form can be defined as follows:

$$Q(u; v, w) := \frac{d}{d\rho}\frac{d}{d\varepsilon}\mathcal{L}(u + \varepsilon v + \rho w)\bigg|_{\varepsilon=0,\rho=0}. \tag{2.15}$$

When the order of differentiation can be interchanged, this form is in fact *symmetric* in v and w:

$$Q(u; v, w) = Q(u; w, v) \tag{2.16}$$

and leads to the introduction of a symmetric mapping $Q(u)$ such that

$$Q(u; v, w) = \int_\Omega v \cdot Q(u)w \equiv \langle v, Q(u)w\rangle. \tag{2.17}$$

This mapping $Q(u)$ is the generalization of the *Hessian matrix* of functions on Euclidian space. It is referred to as the *second variation operator*. Its relation to the second variation is explicitly given by

$$\delta^2\mathcal{L}(u; v) = \langle v, Q(u)v\rangle, \tag{2.18}$$

and in fact, this relation, together with the requirement that Q is symmetric, can serve to define the operator Q.
All these notions can also be translated in statements about the variational derivative $\delta\mathcal{L}$. This is made more precise in the next lemma which will be used frequently in the following.

Lemma 27 *For a functional $\mathcal{L}$ on $\mathcal{M}$, with $\delta\mathcal{L}$ its variational derivative, denote the formal Frechet derivative of $\delta\mathcal{L}$ by $D\delta\mathcal{L}$:*

$$D\delta\mathcal{L}(u)\xi := \frac{d}{d\varepsilon}\delta\mathcal{L}(u + \varepsilon\xi)\bigg|_{\varepsilon=0}. \tag{2.19}$$

Then $D\delta\mathcal{L}(u) : T_u\mathcal{M} \to T_u^*\mathcal{M}$ is a symmetric *map, the* second variation operator*, satisfying*

$$\delta^2\mathcal{L}(u; \xi) =< D\delta\mathcal{L}(u)\xi, \xi >$$

Proof. For arbitrary ξ and η from T_uM it holds

$$\langle D\delta\mathcal{L}(u)\xi,\eta\rangle = \frac{d}{d\varepsilon}\langle\delta\mathcal{L}(U+\varepsilon\xi),\eta\rangle\bigg|_{\varepsilon=0}.$$

Using the definition of variational derivative, this can be rewritten like

$$\langle D\delta\mathcal{L}(u)\xi,\eta\rangle = \frac{d}{d\varepsilon}\frac{d}{d\rho}\mathcal{L}(u+\varepsilon\xi+\rho\eta)\bigg|_{\rho=0,\varepsilon=0}.$$

Assuming smoothness of the function $(\varepsilon,\rho)\to\mathcal{L}(u+\varepsilon\xi+\rho\eta)$, the order of differentiation at the right hand side can be interchanged and one obtains the symmetry as stated.

2.5 Projection of Euler Lagrange equations

In this section, the norm and inner product to be used are the standard L_2 norm and inner product, denoted by

$$\text{norm: } ||u||^2 = \int u(x)^2 dx, \text{ and innerproduct } < f,g >= \int f(x)g(x)dx$$

2.5.1 Projection of functions on finite dimensional subspaces

Let there be given a (finite-dimensional) space of functions, D, explicitly the space of smooth, square integrable functions on the interval $[0,\pi]$, that vanish at the boundary:

$$D = \{u : [0,\pi] \to \mathcal{R}|\ u(0) = u(\pi) = 0\}.$$

Consider, as an example, for integer N, the following finite dimensional subspace of harmonic functions

$$D_N = \left\{\phi = \sum_{k=1}^{N} a_k\sin(kx)|(a_1,...,a_N)\in\mathcal{R}^N\right\}.$$

This space can be identified with the space of coefficients, and so is 'equivalent' to $\mathcal{R}^N$; hence its dimension is N.

1. The projection f_N of a given function $f\in D$ on D_N is defined by

   $$Min_{v\in D_N}||f-v|| = ||f-f_N||$$

   The projection can thus be interpreted as the best approximation (given the norm) of the function f by an element from D_N. Show that it is given by

$$\begin{aligned} f_N(x) &= \sum_{k=1}^{N} \alpha_k \sin(kx), \\ \text{with } \alpha_k &= \frac{< f, \sin(kx) >}{|| \sin(kx)||^2} = \frac{1}{2\pi} < f, \sin(kx) >; \end{aligned}$$

the coefficients are the well known *Fourier-coefficients* (in this case for functions vanishing at the end points).

2. Show that the projection satisfies

   $$< f_N, \sin kx >= \begin{cases} \alpha_k \text{ for } 1 \leq k \leq N \\ 0 \text{ for } k > N \end{cases}$$

3. Prove that

   $$||f_N||^2 = \frac{1}{2\pi} \sum_{k=1}^{N} \alpha_k^2 \leq ||f||^2$$

   and that the difference satisfies

   $$||f - f_N||^2 = \frac{1}{2\pi} \sum_{k=N+1}^{\infty} < f, \sin(kx) >^2$$

   Make graphs to illustrate the meaning of these results.

4. Show that the sets for increasing N are nested as $D_1 \subset D_2 \subset ... \subset D_N$. Show that it is strictly increasing (i.e. that D_{N+1} contains at least one element, actually a whole one-dimensional subspace, that is not in D_N).

5. Taking the limit $N \to \infty$, intuitively means that the finite dimensional space D_N 'approaches' the space D; since

   $$\dim(D_N) = N$$

   this explains why D is called an infinite dimensional space. Show that for each N

   $$||f_N||^2 \leq ||f_{N+1}||^2 \leq ||f||^2,$$

   and hence that $||f_N||^2$ is a sequence that is monotonically increasing, and bounded from above. Show that it follows

   $$\sum_{k=N+1}^{\infty} < f, \sin(kx) >^2 \to 0 \text{ for } N \to \infty$$

   and hence that in the L_2 norm:

   $$f(x) = \lim_{N\to\infty} f_N(x) = \sum_{k=1}^{\infty} \alpha_k \sin(kx)$$

2.5.2 Lagrange's Lemma

If a function f vanishes identically on an interval I , then certainly

$< f, \eta >= 0$ for all functions $\eta : I \to \mathcal{R}$.

The converse is also true, according to Lagrange's Lemma. More precisely, recall the lemma for the simple case of functions on an interval I :

If f is a continuous function on I that satisfies

$< f, \phi >= 0$ for all test functions ϕ on I,

then f is the null function: $f(x) = 0$ for each $x \in I$.

Exercise 28 *1.* Let f be a smooth function on $[-1, 1]$ for which all Fourier coefficients vanish. Then, according to the previous subsection, f is the null function. How is this related to Lagrange's lemma?

2. What can you conclude about a function f for which all Fourier coefficients α_m vanish for $m > N$, for some N ?

3. What can you conclude about a function g for which all Fourier coefficients α_m vanish for $m \leq N$, for some N?

2.5.3 Approximately solving Euler-equations using the direct method

In general, let there be given a bvp consisting of an operator equation (ode or pde), symbolically written $E(u) = 0$, and boundary conditions:

$E(u) = 0$, & boundary cond's.

Suppose the problem is variational, i.e. a functional $\mathcal{L}$ and domain of definition D can be found such that the solutions of the bvp correspond to critical points of $\mathcal{L}$ on D :

$$\text{Crit } \{\mathcal{L}(u) | u \in D\}$$

If we can find these critical point (more easy than the solution of the bvp), we could use this method to find solutions of bvp.
Finding critical points is usually difficult; this is called the direct problem of the Calculus of Variations. But (in particular when the critical point is a minimizer) it may be possible to approximate the critical point by first restricting the functional to a finite dimensional subspace, and then solve the corresponding finite dimensional critical point (minimization) problem. The better (larger) the subspace is taken, the better the critical point can be expected to be approximated; and therefore the better the solution of the bvp can be found.

Exercise 29 Consider for given function f the following bvp

$$-u_{xx} = f(x), \quad u(0) = u(\pi) = 0$$

1. First observe that the exact solution can be obtained by direct integration; write down the solution.

2. Show that the following minimization problem is the corresponding variational formulation:

   $$Min\ \{\mathcal{L}(u) | u \in D\}$$

   with

   $$\mathcal{L}(u) = \int \left[\frac{1}{2}u_x^2 - f(x)u\right] dx, \quad D = \{u | u(0) = u(\pi) = 0\}$$

3. To find a solution of the bvp, one could just as well try to find the minimizer of the variational problem. To do this in an approximate way, suitable finite dimensional subspaces of D should be constructed, on which the functional can be minimized. Construct such suitable subspaces (low dimensional), solve the restricted minimization problem, and compare the approximation with the exact solution, for the following functions f :

   $$f(x) = \begin{array}{l} \cos(x) \\ \sin(x) \\ 1 + x^2 \end{array}$$

Exercise 30 Redo the above exercise, for $f(x) = x$, but now for boundary conditions

$$u(0) = u_x(\pi) = 0$$

We will investigate in the next subsections what the effect is for the Euler-Lagrange equation when the domain of definition of the functional is restricted.

2.5.4 Weak formulation of BVP's

Suppose that U is a solution of the original variational problem

$$U \in Crit\{\mathcal{L}(u) | u \in D\}$$

and hence the desired solution of the BVP. Let D_0 be the set of admissible variations; then it is known that U satisfies

$$\delta\mathcal{L}(U; \eta) = 0, \text{ for all } \eta \in D_0.$$

Assuming no constraints to be present, the set D_0 contains the set of test functions C_0^∞; and then it should certainly hold

$$\delta\mathcal{L}(U; \phi) = 0, \text{ for all } \phi \in C_0^\infty$$

Writing (after partial integrations, if necessary) the variational derivative with the variational derivative, $\delta\mathcal{L}(U;\phi) =< \delta\mathcal{L}(U), \phi >$ there results

$$< \delta\mathcal{L}(U), \phi >= 0, \text{ for all } \phi \in C_0^\infty$$

This means that the projection of (*the function !!*) $\delta\mathcal{L}(U)$ on the set of test functions vanishes; consequently, if $\delta\mathcal{L}(U)$ is continuous, it vanishes (Lagrange's lemma):

$$\delta\mathcal{L}(U) = 0, \text{the Euler-Lagrange (EL-) equation}$$

For the example from the previous subsection

$$\mathcal{L}(u) = \int \left[\frac{1}{2} u_x^2 - f(x)u \right] dx$$

the variational derivative reads

$$\delta\mathcal{L}(U) = -U_{xx} - f(x)$$

and the Euler-Lagrange equation is precisely the requested equation to be solved. The condition $< \delta\mathcal{L}(U), \phi >= 0$, for all $\phi \in C_0^\infty$, or better (to incorporate all boundary conditions), the condition

$$\delta\mathcal{L}(U;\eta) = 0, \text{ for all } \eta \in D_0$$

is often called the *weak formulation* of the corresponding BVP: from this the BVP can be recovered.

2.5.5 Projection of EL-equation from restricting the functional

What happens if we restrict the original domain of definition D of the functional to a smaller set (a finite dimensional subset)? Call the subset $subsD$, and suppose that $V \in subsD$ is the solution:

$$V \in Crit\{\mathcal{L}(v) | v \in subsD\}$$

If $subsD_0$ denotes the corresponding set of admissible variations, then it holds

$$\delta\mathcal{L}(V;\zeta) = 0, \text{ for all } \zeta \in subsD_0$$

Since $subsD_0$ will usually contain a subset of test functions, say $subsC_0^\infty$, this implies

$$< \delta\mathcal{L}(V), \psi >= 0, \text{ for all } \psi \in subsC_0^\infty$$

Since $subsC_0^\infty$ will only be a finite dimensional part of C_0^∞ , we cannot invoke Lagrange's Lemma; the result is merely that the projection of $\delta\mathcal{L}(V)$ on $subsC_0^\infty$ vanishes, and so has at most a component orthogonal to this subset:

$$\delta\mathcal{L}(V) \in (subsC_0^\infty)^{\perp}$$

Conclusion 31 *The function V does not satisfy the EL-equation (in general), but it does satisfy the projection of the EL-equation on the subspace $subsC_0^\infty$.*

Exercise 32 For $D = \{u | u(0) = u(\pi) = 0\}$, take as $subsD$ the 2-dimensional space consisting of harmonic functions

$$subsD = span[\sin(x), \sin(2x)]$$

Make the above explicit in this case for the functional $\mathcal{L}(u) = \int \left[\frac{1}{2}u_x^2 - f(x)u\right] dx$ in the following steps:

1. Find the minimizer on the subspace, the restricted minimizer;
2. Show that the restricted minimizer does not satisfy (in general) the full EL-equation, but does satisfy the projection of the EL-equation on the subset.
3. Can you find a function f for which the restricted has the same solution as the original problem? Explain.
4. What do you expect what will happen with the approximate solution when we increase the subspace by adding more and more harmonic functions.

2.6 Exercises

1. *Calculus for variational derivatives*
   Since functionals map functions into $\mathcal{R}$, functionals can be added and multiplied. Verify the following rules of calculation that are well known for functions on finite dimensional spaces.

$$\begin{aligned} linearity &: \delta(\mathcal{L}_1 + \mathcal{L}_2) = \delta\mathcal{L}_1 + \delta_2; \\ product\ rule &: \delta(\mathcal{L}_1.\mathcal{L}_2) = \mathcal{L}_2\delta\mathcal{L}_1 + \mathcal{L}_1\delta_2; \\ quotient\ rule &: \delta\frac{\mathcal{L}_1}{\mathcal{L}_2} = \frac{\mathcal{L}_2\delta\mathcal{L}_1 - \mathcal{L}_1\delta_2}{\mathcal{L}_2^2} \\ for\ g : \mathcal{R} \to \mathcal{R} &: \delta g(\mathcal{L}) = g'(\mathcal{L})\delta\mathcal{L} \end{aligned}$$

   Derive the corresponding expressions for the second variation.

2. *Inverse problem of the Calculus of Variations*
   The Euler-Lagrange equation of a given functional can be written down. How is it possible to see for a given equation (bvp) if it is the Euler-Lagrange equation of some functional, and if it is, how can we find the functional? This is the “inverse problem” of the Calculus of Variations. The difficulty of the answer depends on the flexibility that is created because one ususally is only interested in the solutions of $\delta\mathcal{L}(u) = 0$. The

flexibility depends on whether transformations (of dependent and/or independent variables) are allowed, because when some flexibility is allowed (multiplication of the equation by a non-vanishing factor), several equations may be found that arise from a suitable functional, as is shown below. In the most strict sense, the answer is a generalization of the conditions that guarantee that a given force field in $\mathcal{R}^n$ is conservative.

(a) A differentiable vector field $F : \mathcal{R}^n \to \mathcal{R}^n$ is called *conservative* if there exists a scalar function $f : \mathcal{R}^n \to \mathcal{R}$ (the so-called potential) such that $F(x) \equiv \nabla f(x)$.
Find the conditions on F that guarantee that it is conservative, and construct the potential directly form F.

(b) Consider for given $n \times n$-matrix the vector field

$$G(x) \equiv (\nabla h)(Ax)$$

where h is a given scalar function. Show that in general G is not conservative.

(c) Consider $g(x) := h(Ax)$, and verify $\nabla g(x) = A^*(\nabla h)(Ax) \equiv A^* G(x)$, where A^* is the adjoint of A. Conclude: if A is invertible, then $\nabla g(x) = 0$ and $G(x) = 0$ have the same solutions. Thus, although G is not conservative, the variational problem for g can be viewed as the variational formulation of the equation $G(x) = 0$.

(d) Derive more generally the relation between the gradients of h and k when they are related by a nonlinear diffeomorphism ψ, i.e.

$$k \equiv h \circ \psi : \quad k(x) = h(\psi(x)) \text{ for all } x.$$

(e) Investigate for given vector function F the critical points of the function $x \mapsto \varphi(|F(x)|^2)$. When are they in a one-to-one relation with the solutions of $F(x) = 0$?

(f) The above can be generalized for functionals. (We restrict to investigate the equation only, forgetting about boundary values).
The operator $u \mapsto E(u)$ is called conservative if there exists some functional $\mathcal{L}$ such that

$$E(u) \equiv \delta\mathcal{L}(u).$$

Let $E'(u)$ denote the formal derivative at the point u. Prove the following result.

Proposition 33 *The operator E is conservative if its derivative defines a symmetric biliniar form, i.e. if*

$$\langle E'(u)\xi, \eta\rangle = \langle \xi, E'(u)\eta\rangle$$

for all functions ξ, η. (Note that we proved that the derivative of the first variation of a functional is symmetric).

If that is the case, the potential functional is given (up to a constant) by

$$\mathcal{L}(u) = \int_0^1 \langle E(su), u\rangle \; ds.$$

(g) If ψ is a smooth transformation of the dependent variables, derive the relation between the variational derivatives of the functional $\mathcal{L}$ and $\mathcal{K}$ related according to

$$\mathcal{L}(u) = \mathcal{K}(\psi(u)).$$

(h) For given operator $E = E(u)$, introduce an arbitrary additonal variable v and consider the functional of the pair (u, v):

$$(u, v) - > \langle E(u), v\rangle \equiv \mathcal{H}(u, v).$$

Derive the Euler-Lagrange equations for $\mathcal{H}$. Conclusion?

3. Consider the following vector fields f on $\mathcal{R}^n$; determine which ones are conservative, and which ones are not. If conservative, write down the potential.

   $n = 2 : f(x, y) = (2x\sin(xy) + x^2y\cos(xy), x^3\cos(xy) + y^3)$

   $n = 2 : f(x, y) = (x^2\sin(y), x^2\cos(y))$

   $n = 3 : f(x, y, z) = (2xy\sin(z) + x^3, x^2\sin(z) + z, x^2y\cos(z) + y)$

4. Find the variational formulation of each of the following boundary value problems:

   $-u_{xx} = \sin(u) + e^x u^2, \;\; u(0) = 0, u_x(1) = 7;$

   $-\frac{1}{r}\partial_r(r\partial_r u) = f(r), \;\; u_r(0) = u(1) = 0;$

   $-div\,[\sigma(x, y)\nabla u(x, y)] + u(x, y) = 0, \quad u(x, 0) = u(x, 1) = u_x(0, y) = u_x(1, y) = 0.$

Chapter 3

Variational structures in Science I

We now present examples of various equations from Mathematical Physics that can be formulated as a variational principle, i.e. the governing equation is the Euler-Lagrange equation of some functional. In many cases, the functional has a clear physical meaning and the optimization problem has physical relevance in itself.

3.1 Geodesic problems

3.1.1 Shortest paths in the plane

Fermat's principle as described in the introduction is one example of a geodesic problem. More generally, such problems deal with curves (in the plane or space) between fixed points P, Q; the curve is sought for which some length functional is as small as possible.
If $n = n(x)$ denotes the weight function, the length functional takes the form

$$\mathcal{L}(\gamma) = \int_\gamma n(x) ds,$$

where γ is the path under consideration, and s is the arc length. Depending on the specific interpretation, the weight n can for instance be:

- the index of refraction (the inverse of the propagation speed) in an inhomogeneous medium for light propagation,
- the cost of a rail connection, depending on the place as a consequence of local soil properties,
- an indication of the presence of obstacles (when $n = \infty$).

The problem of finding the *shortest path* is to find the path $\hat{\gamma}$ such that

$$\hat{\gamma} \in \text{Min } \{\mathcal{L}(\gamma) |\ \gamma \text{ path through } P, Q\}.$$

This can be reformulated by parameterizing the path like $[\tau_0, \tau_1] \ni \tau \mapsto x(\tau)$. Assuming (piecewise) differentiability, and paths in the x, y-plane for instance, the length element

$$ds = |x_\tau| d\tau = \sqrt{x_\tau^2 + y_\tau^2} d\tau$$

leads to the functional

$$\mathcal{L}(x) = \int_{\tau_0}^{\tau_1} \{n(x(\tau) \sqrt{x_\tau^2 + y_\tau^2}\} d\tau$$

which has to be minimized on the set

$$\mathcal{M} = \{[\tau_0, \tau_1] \ni \tau \mapsto x(\tau) \mid x(\tau_0) = P; x(\tau_1) = Q\}.$$

For the particular case that the path can be described as the graph of a function of x, the formulation is

$$\bar{\mathcal{L}}(y) = \int_{x_0}^{x_1} \{n(x, y(x)) \sqrt{1 + y_x^2}\} dx$$

which has to be minimized on the set

$$\bar{\mathcal{M}} = \{[x_0, x_1] \ni x \mapsto y(x) \mid y(x_0) = y_0; y(x_1) = y_1\}$$

where $P = (x_0, y_0), Q = (x_1, y_1)$.

Exercise 34 *1.* Verify that the Euler-Lagrange equations for the functional $\mathcal{L}$ are the two equations

$$\delta_x \mathcal{L}(x) \equiv -\partial_\tau \left[\frac{n(x) x_\tau}{\sqrt{x_\tau^2 + y_\tau^2}} \right] + n_x \sqrt{x_\tau^2 + y_\tau^2} = 0,$$

$$\delta_y \mathcal{L}(x) \equiv -\partial_\tau \left[\frac{n(x) y_\tau}{\sqrt{x_\tau^2 + y_\tau^2}} \right] + n_y \sqrt{x_\tau^2 + y_\tau^2} = 0$$

while for $\bar{\mathcal{L}}$ the Euler-Lagrange equation is

$$\delta \bar{\mathcal{L}}(y) \equiv -\partial_x \left[\frac{n(x, y) y_x}{\sqrt{1 + y_x^2}} \right] + n_y \sqrt{1 + y_x^2} = 0.$$

2. Verify that no natural boundary conditions arise.

3. The equations above are too difficult to solve them explicitly in general. Verify that the optimal path is a straight line if $n \equiv n_0$ is constant. If n depends only on x or only on y, the second order equation can be reduced to a first order equation (see the subsection on "Energy conservation and consequences").

4. Suppose that the points P and Q are on the x-axis, and that the optimal path is a slight deformation of the straight connection (along the x-axis) in the sense that $|y_x|$ is small. Then it can be expected that it is allowed to make the approximation

$$\sqrt{1+y_x^2} \approx 1 + \frac{1}{2} y_x^2$$

and the functional becomes

$$\int \{n(x,y)(1+\frac{1}{2}y_x^2)\}$$

with Euler-Lagrange equation

$$-\partial_x[n y_x] + n_y(1+\frac{1}{2}y_x^2) = 0.$$

Determine the solution in case n only depends on x. What if n only depends on y?

5. Assuming the path to be described as the graph of a function of x, and introducing the angle $\theta(x)$ measuring the tangent direction, the functional becomes

$$\int \frac{n(x,y)}{\cos\theta(x)} dx,$$

where now y has to be related to θ according to

$$y_x = \tan\theta(x), \ \textit{i.e.} \ \ y(x) = y_0 + \int_{x_0}^{x} \tan\theta(\xi) d\xi.$$

Clearly this leads to a minimization problem with a pointwise constraint. When n only depends on x, the problem simplifies to one with an integral constraint:

$$\int_{x_0}^{x_1} \tan\theta(\xi) d\xi = y_1 - y_0;$$

see the next chapter.

3.1.2 Geodetics on Riemmanian manifolds

The above geodetic problems in the plane have a natural generalization to paths of shortest distances on *Riemannian manifold*s. If local coordinates are given by $u = (u^1, \ldots, u^n)$, and the *metric tensor* is $g_{km}(u)$, the arc length is given by

$$ds^2 = g_{km} du^k du^m$$

and the length functional becomes for a parameterized path

$$\mathcal{L}(\gamma) = \int \sqrt{g_{km}(u(\tau))u_\tau^k u_\tau^m} d\tau.$$

For instance, for the unit sphere in $\mathcal{R}^3$, the angle θ and φ are the local coordinates;

$$x = (\cos\varphi \sin\theta, \sin\varphi \sin\theta, \cos\theta)$$

and the metric follows from

$$ds^2 = \sin^2\theta (d\varphi)^2 + (d\theta)^2.$$

3.1.3 Minimal surfaces

Minimal surface of revolution

The graph of a nonnegative function f in the x, y-plane trough two given points when rotated about the x-axis, produces a so-called *surface of revolution.* The area of the surface is given (up to a factor 2π) by

$$\int f(x(s))ds = \int_{x_0}^{x_1} f(x)\sqrt{1+f_x^2}dx$$

and the surface of least area of revolution requires this functional to be minimal.

Soap films

More generally, consider surfaces that are formed by soap films that are spanned between a given prescribed spatial curve.

When the surface can be written as the graph of a function u above the domain Ω in the x, y-plane, and the boundary curve is given by the spatial curve $u(x) = \psi(x)$ for $x \in \partial\Omega$, the surface tension of the soap film will act to minimize the area of the surface, i.e. to minimize the functional

$$\int_\Omega \sqrt{1+|\nabla u|^2}$$

on the set of surfaces through the spatial curve. The Euler-Lagrange equation can be written down:

$$-\text{div}\left[\frac{\nabla u}{\sqrt{1+|\nabla u|^2}}\right] = 0;$$

a solution satisfying the required conditions can mosttimes not be found (if it exist at all!).

When the surface can be expected to be almost straight, say horizontal, the problem can be simplified, just as in the one-dimensional case. Approximating

$$\sqrt{1+|\nabla u|^2} \approx 1 + \frac{1}{2}\nabla u|^2$$

the functional becomes (apart from an inessential constant)

$$\int_\Omega \frac{1}{2}|\nabla u|^2$$

and the Euler-Lagrange equation, including the required boundary condition, leads to a *boundary value problem* for u:

$$\begin{cases} -\Delta u & = 0, \quad \text{in } \Omega \\ u(x) & = \psi, \quad \text{on } \partial\Omega. \end{cases}$$

3.2 Principle of Minimal (Potential) Energy

For time independent problems, or for stationary states of time dependent problems, the actual physical state may be described by a *principle of minimum (potential) energy*, which means the following:

- there is a set of admissible, physically acceptable, states $\mathcal{M}$,
- there is a (potential) energy functional $\mathcal{E}$ that assigns a value ("energy-like") $\mathcal{E}(u)$ to each state $u \in \mathcal{M}$,
- the actual physical state is the state $\hat{u}$ that minimizes $\mathcal{E}$ on $\mathcal{M}$.

We present several examples to illustrate the applicability.

Dirichlet's principle

In a domain $\Omega \subset \mathcal{R}^3$ with an electrostatic field E, the potential energy is $\int_\Omega \frac{1}{2}E^2$. Since rot $E = 0$, the field is conservative: $E = -\nabla\phi$ for an electro-magnetic potential ϕ. In the presence of a charge distribution ρ in the domain, the total electrostatic energy is given by

$$\mathcal{E}(\phi) = \int_\Omega \{\frac{1}{2}|\nabla\phi|^2 - \rho(x)\phi\}dx.$$

Dirichlets principle states that the actual field is such that it minimizes the total energy among all potentials that satify certain boundary conditions.
Two types of boundary conditions are usually considered. When the boundary consists of two parts $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2$, they can be described as

- $\partial\Omega_1$ is conducting, i.e. $E\cdot\tau = 0$ for each tangent vector τ; this is achieved by requiring $\phi = 0$ on the boundary;
- $\partial\Omega_2$ is insulating: $E\cdot n = 0$ on the boundary. This implies that the normal derivative of ϕ vanishes on the boundary $\partial_n\phi = 0$.

The minimization problem

$$\hat{\phi} \in \text{Min } \{\mathcal{E}(\phi) | \phi(x) = 0 \text{ for } x \in \partial\Omega_1\}$$

leads to the boundary value problem

$$\begin{cases} -\Delta\phi &= \rho(x) & \text{in } \Omega, \\ \phi &= 0 & \text{on } \partial\Omega_1, \\ \partial_n \phi &= 0 & \text{on } \partial\Omega_2. \end{cases}$$

Observe that the Neumann condition on $\partial\Omega_2$ arises as a natural boundary condition!
Also note that when $\partial\Omega_1$ is empty (only Neumann conditions) a solution can only exist if $\int \rho = 0$. Inhomogeneous Dirichlet and Neumann boundary conditions can be obtained also: the Dirichlet conditions by prescribing the potential, the Neumann condition by adding a suitable boundary functional to the energy.

Exercise 35 *1.* Show that a critical point of

$$\textit{Crit } \{E(\phi) - \int_{\partial\Omega_2} \psi_2 \phi \mid \phi(x) = \psi_1(x) \textit{ for } x \in \partial\Omega_1\}$$

satisfies

$$\begin{cases} -\Delta\phi &= \rho(x) & \textit{in } \Omega, \\ \phi &= \psi_1 & \text{on } \partial\Omega_1, \\ \partial_n \phi &= \psi_2 & \text{on } \partial\Omega_2. \end{cases}$$

2. Show that there exists at most one critical point, and that,if it exists, it is in fact a minimizer.

3. When $\partial\Omega_1$ is empty, derive the neccessary condition between ψ_2 and ρ for a solution to exist. How is this condition related to the finiteness of the minimum value, i.e. to the boundedness from below, of the functional?

3.2.1 1D-elasticity: bars and strings

An elastic medium is characterized by the fact that deformations from a given rest state require a certain amount of energy. For simplicity we first restrict to 1D elastic media with a rest state along the x-axis, and deformations in a plane. In general, the local energy density will depend on the extension as well as on the curvature of the medium. Two idealizations are

- *strings*: completely flexible, but extension requires energy,
- *bars*: fixed length (inextensible), but bending requires energy.

Theory of bars

For a bar with (fixed) length ℓ it is natural to use the arclength as parameter and to describe its position in the plane as

$$r(s) = (x(s), y(s)), \quad \text{or} \quad r_s(s) = (\cos\theta(s), \sin\theta(s)).$$

The *curvature* $k(s)$ at a point s is defined (up to sign) by

$$k(s) = |r_{ss}|^2 \equiv |\theta_s(s)|^2.$$

The material properties can be described with a local energy density $E = E(s, k(s))$ (depending on position and curvature); in the presence of an external additional potential energy $V = V(r)$, the total energy is then given by

$$\int_0^\ell \{E(s, k(s)) + V(r(s))\} ds.$$

Usually, E is an even function of k and minimal at $k = 0$. Linear elasticity theory (assuming small curvatures) then approximates E like

$$E(s, k) \approx E(s, 0) + \frac{1}{2}\sigma(s)k^2$$

leading to an approximate energy functional

$$\int_0^\ell \{\frac{1}{2}\sigma(s)|r_{ss}|^2 + V(r(s))\} ds,$$

with Euler -Lagrange equation

$$\partial_s^2[\sigma(s)r_{ss}] + \nabla_r V(r) = 0$$

When looking for small vertical deformations u from the rest state along the x-axis, x instead of s is used as the independent variable. (Hence a laboratory coordinate x instead of the material coordinate s; note that then, with $x \in [0, \ell]$, the bar slightly extends.) If f is a prescribed vertical force ($\approx \partial_y V(x, 0)$), the resulting energy functional becomes

$$\int_0^\ell \{\frac{1}{2}\sigma(x)u_{xx}^2 - f(x)u(x)\} dx.$$

The Euler-Lagrange equation reads

$$\partial_x^2[\sigma u_{xx}] = f(x), \text{ for } x \in (0, \ell).$$

Concerning boundary conditions, two types can be distinguished:

- *supported endpoint*: only the position is prescribed, for instance $u(0) = 0$;
- *inclined endpoint*: a more restricted condition for which both the position and the angle are prescribed, for instance $u(0) = 0, u_x(0) = 1$.

When a bar is supported at one endpoint, say $x = 0$, a natural boundary condition arises in addition to the prescribed position:

$$u(0) = 0, \quad \sigma(0)u_{xx}(0) = 0;$$

at an inclined end point, no natural boundary conditions arise.

Theory of strings
In a string, both longitudinal and transvers displacements of particles will occur. If one restricts to small deflections form a state of rest along the x-axis, the change in length is in lowest order given by

$$[\sqrt{1+u_x^2} - 1]dx \approx \frac{1}{2}u_x^2.$$

With $\sigma(x)$ the tension in the undeformed state, and f an external vertical force, the approximated potential energy is given by

$$\int_0^\ell \{\frac{1}{2}\sigma u_x^2 - f(x)u\}dx,$$

leading to the Euler-Lagrange equation

$$-\partial_x[\sigma(x)u_x] = f(x) \text{ for } x \in (0,\ell).$$

When the deflection is not prescribed at an end point, a natural boundary condition appears: $\sigma u_x = 0$.

3.2.2 2D-elasticity: plates and membranes

2D elasticity is a direct generalization of the 1D elastica; in the linear approximation, the analog of a bar is a plate and has potential energy

$$\int_\Omega \{\frac{1}{2}\sigma(\Delta u)^2 - f(x)u\}dx;$$

the analog of a string is a membrane, with approximate potential energy

$$\int_\Omega \{\frac{1}{2}\sigma|\nabla u|^2 - f(x)u\}dx.$$

Boundary conditions, prescribed and natural boundary conditions, can be of the same type as in the 1D case.

3.3 Dynamic variational principles

We now come to dynamical systems with the property that their *evolution* satisfies a certain optimality; so not just one state, but the whole evolution between certain specified initial and final times.
In the special case that such systems are in an equilibrium state (no motion), it is usually the case that this equilibrium state satisfies a principle of minimal

potential energy as treated above. But the peculiar fact is now that each (possible) dynamic evolution admits a variational description.
We treat two classes, Lagrangian and Hamiltonian systems; it will be shown later that in several cases (in particular for systems from Classical Mechanics and continuum mechanics) one physical system can be described in either way, with a Legendre transformation connecting the different descriptions.

3.3.1 Lagrangian systems

Let Q be the so-called *configuration space* of a dynamical system. For discrete systems, Q will be a subset of $\mathcal{R}^N$, denoting the set of (generalized) coordinates that describe the position in space of the system. For continuous systems, Q will be some (subset of a) function space.

If we denote a particular state by $u(t) \in Q$, and the evolution as a trajectory $t \mapsto u(t) \in Q$, the velocity can be interpreted as an element form the tangent space:

$$\partial_t u \in T_u Q.$$

A *Lagrangian* is a function(al) defined on the tangent space:

$$L : \mathcal{R} \times Q \times T_Q \in \mathcal{R}, \quad L = L(t, u, v),$$

with the aid of which a so-called *action functional* can be defined: for evolutions $t \mapsto u(t)$ with $t \in [t_0, t_1]$

$$\mathcal{A}(u) = \int_{t_0}^{t_1} L(t, u(t), \partial_t u(t)) dt.$$

Definition 36 *A dynamical system is called a* Lagrangian system *if a Lagrangian can be defined as above such that the actual evolutions of the system are critical points of the corresponding action functional.*

Describing Lagrangian systems as the critical points of an action functional is called the *action principle*. In general the evolutions are not minimizers of the action functional, but only saddle points.

To find the evolution equations for a specific system, it is important to be aware of the following.

Observation: In many problems form classical and continuous mechanics, *the Lagrangian is the difference of kinetic and potential energy*, both expressed in terms of the variables from configuration space.

It should also be remarked that no boundary conditions at t_0 and t_1 are mentioned; the dynamic variational problem above is just meant to produce the correct set of equations, i.e. the Euler-Lagrange equation of the action functional.

The Euler - Lagrange equation reads in a somewhat imprecise, but rather clear and common, way

$$-\partial_t \left[\frac{\partial L}{\partial_t u}\right] + \frac{\partial L}{\partial u} = 0.$$

Note that when Q is infinite dimensional, for continuous systems, the Lagrangian itself is a functional (over the spatial domain, of the two variables u, v), and the derivatives with respect to these variables are to be interpreted as variational derivatives (with the spatial inner product). We will see specific examples in the following.

The *simplest problem in the Calculus of Variations* is the following.
Using the notation of classical mechanics, let $q \in \mathcal{R}^N$ be a coordinate vector, measuring the position of a discrete system. Since now $Q = \mathcal{R}^N$, the tangent space is simply $TQ = \mathcal{R}^N$ at each point. With a Lagrangian function on $\mathcal{R}^{2N+1}$ depending on $t \in \mathcal{R}, q \in \mathcal{R}^N$ and ("velocity") $v \in \mathcal{R}^N$: $L[q](t) \equiv L(t, q(t), \dot{q}(t))$, the action functional reads

$$\mathcal{A}(q) = \int_{t_0}^{t_1} L[q](t)dt. \tag{3.1}$$

Using the abbreviations $L_v = \partial L/\partial v,\ L_q = \partial L/\partial q$, the Euler-Lagrange equations are given by

$$-\frac{d}{dt}[L_v[q]] + L_q[q] = 0. \tag{3.2}$$

These are N differential equations, second order in time in general.
As a specific example, take

$$L(q, v) = \frac{1}{2} v \cdot Mv - V(q) \tag{3.3}$$

Then the resulting Euler-Lagrange equation is precisely Newton's equation (with M the mass matrix and V the potential energy):

$$\frac{d}{dt}[M\dot{q}] = -\partial_q V(q). \tag{3.4}$$

The corresponding *action principle for continuous systems* is described by functions $u = u(x, t)$ with spatial variable $x \in \Omega_0 \subset \mathcal{R}^n$. Let $\rho(x)$ be a given positive mass-density, and V the potential energy considered as a functional of functions on Ω_0, i.e. $V(u) = \int_{\Omega_0} W[u]dx$. Then take as action functional the difference of kinetic and potential energy:

$$\mathcal{A}(u) = \int dt[\int_{\Omega_0} \frac{1}{2}\rho(x)u_t^2 dx - V(u)]. \tag{3.5}$$

The Euler-Lagrange equation can be written as

$$\rho(x)\partial_t^2 u = -\delta_u V(u) \tag{3.6}$$

where $\delta_u V(u)$ denotes the variational derivative of V with respect to functions on the spatial domain Ω_0.

For instance, for the specific choice (σ is a given positive function on Ω_0, and f a given function depending on u and possibly x)

$$V(u) = \int (\frac{1}{2}\sigma(x)|\nabla u|^2 + f(u)), \tag{3.7}$$

the variational derivative is given by

$$\delta_u V(u) = -\text{ div } (\sigma(x)\nabla u) + \frac{df(u)}{du},$$

and the Euler-Lagrange equation reads

$$\rho(x)\partial_t^2 u = \text{ div } (\sigma(x)\nabla u) - \frac{df(u)}{du}. \tag{3.8}$$

This is a (nonlinear) wave equation. When, ρ and σ are constant, and $f \equiv 0$, the equation is the simple wave equation

$$\partial_t^2 u = c^2 \Delta u$$

with $c^2 = \sigma/\rho$ and Δ the Laplace operator.

3.3.2 Hamiltonian systems

Hamiltonian systems are systems that can also be found from a variational principle: the *canonical action principle*.

Now the description is on the cotangent space T^*Q of the configuration manifold. With $q \in Q$ ("position") and $p \in T_q^*Q$ ("momentum") as variables, the state of the system is described by the pair (q,p); this is often called the *phase space*. A *Hamiltonian* is a function(al) on the cotangent space:

$$H : \mathcal{R} \times Q \times T_Q^* \to \mathcal{R}, \quad H = H(t,q,p).$$

A so-called *canonical action functional* is defined for evolutions $t \mapsto (q(t), p(t))$ with $t \in [t_0, t_1]$

$$\mathcal{A}_c(q,p) = \int_{t_0}^{t_1} [< p(t), \partial_t q(t) > -H(t, q(t), p(t))]\, dt.$$

Definition 37 *A dynamical system is called a* Hamiltonian system *if a Hamiltonian can be defined as above such that the actual evolutions of the system are critical points of the corresponding canonical action functional.*

Describing Hamiltonian systems as the critical points of a canonical action functional is called the *canonical action principle*.

To find the evolution equations for a specific system, it is important to be aware of the following.

Observation: In many problems form classical and continuous mechanics, *the Hamiltonian is the sum of kinetic and potential energy, i.e. the total energy*, both expressed in terms of the canonical variables from the phase space.

Hamilton's equations for a system with Hamiltonian H are the Euler-Lagrange equations of the canonical action functional; they are readily found to be

$$\left\{ \begin{array}{lcl} \partial_t q & = & \frac{\partial H}{\partial p} \\ \partial_t p & = & -\frac{\partial H}{\partial q} \end{array} \right. \tag{3.9}$$

with some careful interpretation of the notation (the partial derivatives are variational derivatives of the Hamiltonian functional for continuous systems).

Exercise 38 *1.* As a specific example of a finite dimensional system, verify that Newtons equations as given above, are also obtained for

$$H(q,p) = \frac{1}{2} p \cdot M^{-1} p + V(q)$$

2. For plane fluid motions, the velocity field $v(x,y)$ can be written with a streamfunction ψ when the flow is irrotational like

$$v(x,y) = (\psi_y, -\psi_x).$$

Observing that the fluid velocity is the particle velocity,

$$v(x,y) = (\partial_t x, \partial_t y),$$

it is clear that the particle dynamics is a Hamiltonian system.

Example 39 For a continuous system on a spatial domain Ω, and with $q = q(x,t), p = p(x,t)$ the canonical variables, the canonical action principle is

$$\mathcal{A}(q,p) = \int [\int_{\Omega_0} p \partial_t q dx - H(q,p)] dt. \tag{3.10}$$

With a Hamiltonian that is the sum of potential and kinetic energy:

$$H(q,p) = \int_{\Omega_0} \frac{1}{2\rho} p^2 dx + V(q), \tag{3.11}$$

the Hamiltonian system evolves according to

$$\begin{cases} \partial_t q & = & \frac{1}{\rho} p \\ \partial_t p & = & -\delta V(q), \end{cases}$$

equivalent with the continuous version of Newton's equation:

$$\rho \partial_t^2 q = -\delta V(q).$$

3.3.3 Energy conservation and consequences

The dynamical systems considered above turn out to be "energy"-conserving when they are autonomous. This result is stated here for both Lagrangian and Hamiltonian systems separately; later we will be able to see the connection when these two classes are related by a Legendre transformation.

Proposition 40 *For an autonomous Hamiltonian system, i.e. the Hamiltonian $H = H(q,p)$ does not depend explicitly on t, H is conserved during the evolution:*

$$\partial_t H(q(t), p(t)) = 0 \text{ for all solutions };$$

this means that the dynamics in the state space is confined to the level set of H determined by the initial condition. It is said that H is a first integral*, or constant of the motion. Since H is often energy, this is referred to as "energy conservation", and the system is called conservative.*
For an autonomous Lagrangian system, i.e. the Lagrangian $L = L(q,v)$ does not depend explicitly on t, the following quantity $E(q,\dot{q})$ is conserved during the evolution:

$$\partial_t E(q,\dot{q}) = 0, \text{ with } E(q,\dot{q}) = \dot{q}\frac{\partial L}{\partial \dot{q}} - L(q,\dot{q}).$$

This quantity E is a first integral*; since often this quantity is the total energy, this is referred to as "energy conservation", and the system is called conservative.*

Be aware of the notation! The result holds for infinite dimensional systems just as well as for finite dimensional systems.

Exercise 41 Prove the proposition above.

For problems with one degree of freedom, i.e. $q \in \mathcal{R}$ for Lagrangian systems, and $(q,p) \in \mathcal{R}^2$ for Hamiltonian systems, the energy conservation above actually "solves" the problem: the trajectories of the dynamics in the phase plane $(q,\dot{q})$ or (q,p) are implicitly defined by the level lines of E, resp. H. For a Lagrangian system, "solving" the equation $E(q,\dot{q}) = E_0$ for $\dot{q}$ provides a first order differential equation for q: the second order differential equation is transformed to a first order equation (that depends on the value of the energy E_0 determined by the initial condition). This observation sometimes make it possible to solve several problems; see below.

Exercise 42 Use the observation about energy conservation to "solve" the following problems, that is to make a phase plane analysis (determine equilibrium solutions, sketch trajectories) and, in special cases, to find the solution in elementary functions.

1. The Lagrangian system with $L(q,v) = \frac{1}{2}mv^2 - V(q)$, where $m > 0$ and V is given below. (First find the expression for E.)
    (a) $V(q) = \frac{1}{2}q^2$ (harmonic oscillator);
    (b) $V(q) = 1 - \cos q$ (pendulum equation);
    (c) $V(q) = \frac{1}{2}q^2 - q^4$;
    (d) $V(q) = \frac{1}{2}q^2 - q^3$.
2. The Hamiltonian system with $H(q,p) = \frac{1}{2m}p^2 + V(q)$, with V as given above; relate H with the expression E found above.
3. The geodesic problem in the plane with length functional $\int n(x,y)\sqrt{1+y_x^2}dx$ when n does not depend on x explicitly. Consider the special case $n = y$ and $n = \frac{1}{y}$ for which the trajectories can be expressed explicitly.
4. *Momentum-type of first integrals*
   Assume that, for an n-dimensional configuration space, the Lagrangian L does not depend on one of the coordinates, say q_1 (in that case it is said that q_1 is a "cyclic" coordinate). Show that then one of the Euler-Lagrange equations leads immediately to a first integral:

   $$\partial_t P_1(q,\dot{q}) = 0, \quad \text{with} \quad P_1 = \frac{\partial L}{\partial \dot{q}_1}.$$

   In classical mechanics, P_1 can often be interpreted as a momentum-like quantity.

    (a) Find an analogous property for Hamiltonian systems for which one coordinate is cyclic.
    (b) Use this result to study the geodesics problem with $n = n(x)$.
    (c) Study the motion of a mass point moving in the plane under the influence of a central force (depending on the distance to the origin only); use polar coordiantes to describe the motion; the Lagrangian is the difference of kinetic and potential energy. Observe the two first integrals: the energy and the angular momentum!

3.4 Description of continua in Lagrangian variables

In this section we describe general continua by a direct generalization of finite dimensional particle systems; the description found is the so-called material description of continua.

3.4.1 Canonical Hamiltonian systems

A general and important example of an infinite dimensional Poisson system is the direct generalization of a finite dimensional canonical Hamiltonian system. It is formulated as follows.

Let $\Omega_0 \subset \mathcal{R}^n$ and let $\mathcal{U}$ be a linear space of pairs of d-vector functions defined on Ω_0:

$$\mathcal{U} = \{u = (q,p) : \Omega_0 \to \mathcal{R}^d \times \mathcal{R}^d\}$$

When the elements of Ω_0 are denoted by $\xi \in \Omega_0$ they can be interpreted as a continuous variable "labeling" the particles for which $q(\xi,t)$ is the position and $p(\xi,t)$ the momentum.
The variational derivative of a functional F, $F(u) = F(q,p)$, will be written as

$$\delta_u F(u) = \begin{pmatrix} \delta_q F \\ \delta_p F \end{pmatrix} \tag{3.12}$$

where $\delta_q F$ and $\delta_p F$ denote the partial variational derivatives of F with respect to q and p respectively. Then one has the following direct generalization of Hamiltons equations for a system with Hamiltonian H, namely

$$\partial_t u = J\delta_u H(u), \text{ with } J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{3.13}$$

which can be written in the components q and p as

$$\left\{ \begin{array}{rcl} \partial_t q & = & \delta_p H(q,p) \\ \partial_t p & = & -\delta_q H(q,p) \end{array} \right. . \tag{3.14}$$

Remark 43 *Just as for discrete systems, Hamilton's equations for continuous systems can be found as the Euler-Lagrange equations of a canonical action functional:*

$$\mathcal{A}(q,p) = \int [\langle p, \partial_t q\rangle - H(q,p)]dt.$$

The equations (3.13) are a direct generalisation of (**??**) upon replacing the summation over the integers $k, 1 \leq k \leq n$, labeling N discrete particles, by an integration over the continuous labels ξ. Correspondingly it should be observed that the time derivative as it appears here is the *material time-derivative*: the derivative at fixed particle.
Describing a continuum in this way is called the *material description*, or *Lagrangian description*. Often, the position of a particle at some initial time $t = 0$ is taken as the label ξ. Then $q(\xi,t)$ maps the initial configuration into the configuration at time t.
In a *Eulerian description*, laboratory coordinates (spatial variables x and time t) are the independent variables, and the label $\xi = \xi(x,t)$ and the Eulerian velocity

$v = v(x,t)$ are the dependent variables. The (time-dependent) transformation between the Lagrangian and Eulerian description is given by

$$q(\xi(x,t),t) = x, \quad p(\xi(x,t),t) = v(x,t).$$

Since (**??**) is the basic bracket for the material description of a continuum, it will be called the *canonical continuum description*[1].

3.4.2 Continuous Lagrangian systems

Analogously to the role that Lagrangian systems play in Classical Mechanics, Hamiltonian systems defined on the cotangent space of a configuration manifold are particularly important in Continuum Mechanics. If Q is the configuration manifold, consider the cotangent space

$$\mathcal{M} = T^*Q = \{(q,p) \mid q \in Q, p \in T_q^*Q\}. \tag{3.15}$$

Second order Hamiltonian systems are obtained from a natural Hamiltonian which is of the form

$$H(q,p) = \frac{1}{2}\int_{\Omega_0} \rho_0^{-1}(\xi)p^2 d\xi + \bar{V}(q) \tag{3.16}$$

where ρ_0 is a given "mass"-density (a positive function), and where $\bar{V}$ is a potential energy functional. Then Hamilton's equations

$$\left\{\begin{array}{lcl} \partial_t q & = & \rho_0^{-1}(\xi)p \\ \partial_t p & = & -\delta_q \bar{V}(q) \end{array}\right. \tag{3.17}$$

can be written as the following continuous variant of Newton's equations:

$$\rho_0(\xi)\partial_t^2 q = -\delta_q \bar{V}(q). \tag{3.18}$$

Exercise 44 *1.* To describe the longitudinal motions in an elastic string, it can be modelled as a continuum limit of a number of mass points that can move along the x-axis. With $q = q(\xi,t)$ the position function, in the simplest case the potential energy function depends on the derivative q_ξ only. Derive the equations of motion for potential energy function $V(q_\xi)$.

2. Specialize the equation for $\rho(\xi) \equiv 1$, and V quadratic.

3. In the general case, introduce as new variable, to replace $q(\xi)$, the variable $\ell(\xi)$ (the "specific length", the inverse of the mass-density) that is related to q by $\ell(\xi) = q_\xi(\xi)$. Derive the (Hamilton) equations using this variable ℓ as one of the variables.

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[1] For finite dimensional systems the word "canonical" refers to the implication of Darboux' theorem that (under some conditions) each Poisson system can be written locally as a Hamiltonian system with the special canonical structure. In infinite dimensions, no generalisation of Darboux' theorem exists. The use of the word *canonical* in the infinite dimensional case refers to the important role (**??**) plays for continuous systems.

3.5 Exercises

1. *Linear two-point boundary value problem*
   For given $f \in C^0([0,1])$ consider

$$\mathcal{L}(u) = \int_0^1 \{\frac{1}{2}u_x^2 - f(x)u\}dx.$$

   (a) Prove: $\hat{u} \in C^2$ is a solution of the bvp

$$\begin{cases} -u_{xx} = f & \textit{on } (0,1) \\ u(0) = u_x(1) = 0 \end{cases}$$

   iff $\hat{u}$ is the only critical point of $\mathcal{L}$ on

$$M_0 = \{u \ \text{ piecewise differentiable} \mid u(0) = 0 \ \};$$

   in fact it is a minimizer for $\mathcal{L}$ on this set. (Concerning additional regularity for a critical point, see also the next Chapter, the Exercise on "Lemma DuBois-Reymond, Integrated Euler-Lagrange equation".)

   (b) Show that for the Neumann problem

$$-u_{xx} = f, \quad u_x(0) = u_x(1) = 0,$$

   there exists a solution iff $\int_0^1 f(x)dx = 0$. If it exists, the solution is not unique. Moreover show that

   - if $\int_0^1 f(x)dx = 0$, $\hat{u}$ is a solution iff it is a minimizer (not isolated) of $\mathcal{L}$ on the set of piecewise differentiable functions (no restrictions on the boundary);
   - if $\int_0^1 f(x)dx \neq 0$, $\mathcal{L}$ does not have a critical point on the set of piecewise differentiable functions (no restrictions on the boundary); the infimum of this functional is $-\infty$.

2. *Nonlinear two-point boundary value problem*
   For given $f \in C^1([0,1] \times \mathcal{R}, \mathcal{R})$ consider the non linear bvp

$$\begin{cases} -u_{xx} \ = \ f(x,u) & \text{on } \ (0,1) \\ u(0) = u(1) = 0 \end{cases}$$

   (a) Give the variational formulation, i.e. the functional $\mathcal{L}$ such that its critical points on $M_0 = \{u \mid u(0) = u(1) = 0\}$ correspond to the solutions of the bvp.

   (b) Determine the second variation: $\eta \mapsto \delta^2\mathcal{L}(u;\eta) \equiv Q_u(\eta)$.

   (c) Write down the Euler-Lagrange equation for $\eta \mapsto Q_u(\eta)$.

   (d) Compare the result with the *linearization* of the bvp:

$$\begin{cases} -\eta_{xx} \ = \ f'(x,u)\eta & \text{on } \ (0,1) \\ \eta(0) = \eta(1) = 0 \end{cases}.$$

(e) Show that if the linearized bvp has a nontrivial solution $\hat{\eta}$, then $Q_u(\hat{\eta}) = 0$.

(f) Prove the general result:

Proposition 45 *The linearization of the Euler-Lagrange equation of a functional $\mathcal{L}$ around a solution u is the Euler-Lagrange equation of the second variation $\delta^2\mathcal{L}(u;\cdot)$.*

3. *Euler buckling*
Reconsider the transversal deflections of a bar, written with the arclength s, and angle $\theta = \theta(s)$. Assume that in the rest state the bar is along the x-axis, length ℓ, and fixed at $x = 0$. The other end point is free. Take for the bending energy (related to the curvature θ_s)

$$\int_0^\ell \frac{1}{2}\theta_s^2 ds.$$

If at the free end point a force μ is acting in the direction of the negative x-axis, then $\mu[\ell - x(\ell)]$ is the work executed by the force. For given force, the deflection is described by the principle of minimal potential energy, i.e. of the funtional

$$\mathcal{L}(\theta) = \int_0^\ell \{\frac{1}{2}\theta_s^2 - \mu(1 - \cos\theta)\} ds.$$

(a) Determine the bvp for a critical point. What is the meaning of the (natural) boundary condition at $s = 0$ and $s = \ell$.

(b) Relate the equation to that for the pendulum equation

$$\ddot{x} = -\sin x;$$

which dynamic solutions correspond to the desired deflection of the bar? Use "energy-conservation" to write down the solution implicitly.

(c) To investigate the Euler-buckling problem directly, observe that with a solution $\theta(s)$, also $-\theta(s)$ is a solution, and hence $\theta \equiv 0$ is a solution for all μ.

(d) Determine the second variation around the trivial state, and show that only for specific values of $\mu = \mu_k$, $k \in \mathbb{N}$, the linearized equation has nontrivial solutions, and determine these solutions. Verify that all these solutions correspond to the same physical oscillation of the linearized pendulum equation.

(e) Conclude from the phase plane analysis of the pendulum equation that for the Euler buckling there is a *bifurcation value* μ_1 such that for $\mu < \mu_1$ there is no nontrivial buckled state, while for any $\mu > \mu_1$ there is precisely one buckled state that is positive.

4. *Periodic motions and boundary conditions*
We have already remarked that in general the dynamic variational principles are not well suited to prove existence; ususally dynamic evolutions are saddle points of the action functional. In particular cases existence can be proved with variational methods. The most succesful results deal with period solutions, the reason being that then the problem can be formulated as a boundary value problem. We will show that in this exercise. Consider a Lagrangian dynamical system with Lagrangian L. L may depend on t, but if it does, it is in a periodc way, say with period T. Then one may look for motions that are periodic with period T.

   (a) Show that the evolution $t \mapsto q(t)$ is T-periodic iff it is the periodic continuation of the function defined on $[0, T]$ that satisfies the *periodic boundary conditions*:
   $$q(0) = q(T), \quad \dot{q}(0) = \dot{q}(T).$$

   (b) Show that (under mild assumptions) these boundary conditions arise partly as natural boundary conditions from the action functional with prescribed boundary condition for q only: $q(0) = q(T)$.

   (c) Formulate the periodic boundary conditions for a Hamiltonian system; show that they arise from the canonical action principle when only conditions on q are prescribed as above.

5. *Jacobi functional* in Classical Mechanics
For a Lagrangian system for which the energy is conserved, one may look for solutions of prescribed total energy E.

   (a) Consider the Jacobi functional on the set of functions $[0, 1] \ni \tau \mapsto x(\tau) \in \mathcal{R}^n$ with $x(0) = x(1)$:
   $$J(x) = \int_0^1 \sqrt{E - V(x)}|x_\tau| d\tau$$
   Derive the equation for its critical points, and the boundary conditions.

   (b) Show that for a suitable scaling of the parameter τ to t and a related transformation $x(\tau) \equiv q(t)$, a standard second order Newton equation for q and potential V results; show that the solution has indeed energy E. What about the boundary conditions?

   (c) How can the Jacobi functional be obtained by constraining the action principle to motions that satisfy the energy constraint?

   (d) Show that the following *modified Jacobi functional* can serve the same purposes:
   $$[\int_0^1 \dot{x}^2 d\tau] \ . \ [E - \int_0^1 V(x) d\tau].$$
   How can this functional be obtained form the action principle and an energy constraint?

6. *Stationary states of a nonlinear diffusion equation*
   Consider the stationary solutions of a nonlinear diffusion equation on a domain Ω for which the diffusion coefficient D may depend on u:

$$\left\{ \begin{array}{rcll} \mathrm{div}\ [D(u)\nabla u] + f(x,u) & = & 0 & in\Omega \\ u(x) & = & \varphi(x) & on\partial\Omega_1, \\ D(u)\frac{\partial u}{\partial n} & = & \psi(x) & on\partial\Omega_2. \end{array} \right.$$

   (a) When D is constant derive the variational formulation of this boundary value problem (including the boundary conditions).

   (b) Observe that when D depends on u there is no obvious variational formulation.

   (c) Suppose that D is positive and a monotone function of u. Consider the transformation of the dependent variable $u \to v$ such that

$$\nabla v = D(u)\nabla u.$$

   Show that v can be expressed directly in terms of u.

   (d) Derive the governing boundary value problem for v.

   (e) Show that the bvp for v has a variational structure; denote the governing functional by $\mathcal{L} = \mathcal{L}(v)$.

   (f) Define uniquely the functional $\bar{\mathcal{L}}$ of u as

$$\mathcal{L}(v) \equiv \bar{\mathcal{L}}(u).$$

   Find the critical points of $\bar{\mathcal{L}}(u)$. Verify the transformation between the two formulations of the boundary value problem from relations between $\delta_v \mathcal{L}(v)$ and $\delta_u \bar{\mathcal{L}}$.

   (g) Conclusion?

7. *Variations of the boundary*
   Consider (for simplicity, on the plane) a given density function ρ and the total "mass" in a region Ω:

$$M(\Omega) = \int_\Omega \rho(x,y)dxdy.$$

   We want to see how M depends on Ω. (Assume that the regions are "convex-like" and can be deformed smoothly without introducing intersections.)

   (a) First take the special case that Ω is the area between the x-axis and the graph of a function $\eta = \eta(x)$:

$$\Omega = \{\ (x,y)\ \mid\ a \le x \le b,\ 0 \le y \le \eta(x)\ \},$$

and consider the corresponding functional

$$\mathcal{L}(\eta) = M(\Omega).$$

Determine the first variation and show that the variational derivative of $\mathcal{L}$ for variations of the domain described by a variation of the function η is given by

$$\delta\mathcal{L}(\eta) = \rho\mid_{y=\eta(x)} \equiv \rho(x, \eta(x)).$$

(b) Now, more generally, descibe a variation of the boundary $\partial\Omega$ by a "normal" displacement σ (defined on the boundary). Determine the first variation of M.
Can you find an expression for the variational derivative of M?
Verify the formula for the case of a radial deformation of a circular domain (and $\rho = 1$).

(c) Show that the more general result specializes to the case of changing the graph that determines the boundary. (Relate a variation η and the normal displacement σ in this case.)

Chapter 4

Constrained variational problems

4.1 Geometry of nonlinear manifolds

Many variational problems that are encountered deal with *constrained variational problems.* This means that, besides certain boundary conditions, the functions belonging to the set of admisible elements $\mathcal{M}$ also satisfy certain "interior" conditions. Then, if u belongs to $\mathcal{M}$, for a variation $\eta \in C_0^\infty(\Omega)$, the function $u + \varepsilon\eta$ does *not* in general belong to $\mathcal{M}$ (up to second order): the set $\mathcal{M}$ is a nonlinear manifold. Stated in a different way, the tangent space does not contain all test functions:

$$C_0^\infty(\Omega) \not\subset T_u\mathcal{M}.$$

In the problems to follow, the manifolds $\mathcal{M}$ will be subsets of a function space $\mathcal{U}$ for which the functions satisfy (apart from certain boundary conditions) a finite number of nonlinear *functional constraints*.

To deal with (linear) inhomogeneous boundary conditions in a decent way in the following requires some precautions. Therefore, let $\mathcal{U}$ be the space of functions satifying the (linear) boundary conditions, and let $\mathcal{U}_0$ be the tangent space to $\mathcal{U}$, i.e. $\mathcal{U}_0$ consists of elements v such that $u + \varepsilon v \in \mathcal{U}$ whenever $u \in \mathcal{U}$: v are the functions that satisfy the homogeneous boundary conditions.

In most of the following, the set $\mathcal{M}$ of admissible elements will be defined as the intersection of the levelsets of certain (density) functionals $\mathcal{K}_1, \ldots, \mathcal{K}_p$:

$$\mathcal{M} \;=\; \{\; u \in \mathcal{U} \;\mid\; \mathcal{K}_1(u) = k_1, \ldots, \mathcal{K}_p(u) = k_p \;\}, \tag{4.1}$$

where $k_1, \ldots, k_p$ are given values. In general this set may be empty, so we assume that for the given values of the constraints $k_1, \ldots, k_p$ this set is non-empty.

When extremizing a functional $\mathcal{L}$ on a set $\mathcal{M}$, we arrive at the stationarity condition for a critical point:

$$\delta\mathcal{L}(\hat{u}; v) = 0 \text{ for all } \; v \in T_{\hat{u}}\mathcal{M},$$

as derived in the previous chapter. To investigate this further, we need to know the tangent space of the set $\mathcal{M}$.

4.1.1 Regular points of the manifold

Roughly speaking, one can distinguish between regular and singular points on $\mathcal{M}$. In the regular points, the p constraints define a tangent space that contains all but p directions, and the set $\mathcal{M}$ near a regular point is well approximated by a linear space (hyper plane) of codimension p, the analog of a $(n-p)$-dimensional smooth manifold in $\mathcal{R}^n$. Stated differently, at a regular point, there are p independent normal directions to the tangent space.
In a singular point, some of the normal directions to the tangent space coincide: the elements of the tangent space are restricted by less than p conditions. We will make this more precise in the following.

Definition 46 *A point* $u \in \mathcal{M}$ *is called a* regular point *of the manifold* $\mathcal{M}$ *if the linear functionals* $\delta\mathcal{K}_1(u;\cdot), \ldots, \delta\mathcal{K}_p(u;\cdot)$ *are linearly independent for* $u \in \mathcal{M}$. *A* singular point *is a point of* $\mathcal{M}$ *that is not regular.*

The linear independence of the linear functionals can be expressed in a different way by using the variational derivatives. Since $\delta\mathcal{K}(u;\eta) =< \delta\mathcal{K}(u), \eta >$, for $\eta \in C_0^\infty \subset \mathcal{U}_0$, the following holds.

Proposition 47 *The independence of the linear functionals*

$$\delta\mathcal{K}_1(u;\cdot), \ldots, \delta\mathcal{K}_p(u;\cdot) \text{ on } \mathcal{U}_0$$

implies the indepence of the p *variational derivatives (as elements of* $L_2(\Omega)$*)*

$$\delta\mathcal{K}_1(u), \ldots, \delta\mathcal{K}_p(u).$$

Exercise 48 In finite dimensions $\mathcal{R}^n, n > 1$ consider the following simple examples.

1. For $n = 2$, the levelsets of a function $K = K(x, y)$ are curves in the plane. A regular point $u = (x, y)$ is one for which $\nabla K(x, y) \neq 0$; the singular points are those for which $\nabla K(x, y) = 0$.
   At a regular point, the tangent "space" is the one-dimensional straight line through the point in the tangent direction: the direction vector τ such that $\nabla K(x, y) \cdot \tau = 0$. Hence $\nabla K(x, y)$ is the normal to the tangent line, i.e. normal to the level line.
   For instance, for $K(x, y) = x^2 + y^2$, every point on the level set $K^{-1}(k)$ with $k > 0$ is a regular point; for $k = 0$, the point $(0, 0)$ (which is the only point on the level set) is singular.

2. In $\mathcal{R}^3$, consider the intersection of a sphere with a horizontal plane:

$$\mathcal{M} = \{ \ (x, y, z) \ \mid \ x^2 + y^2 + z^2 = R^2, \ z = \zeta \ \}.$$

   When $|\zeta| < R$, each point is a regular point and the tangent space is one-dimensional; when $\zeta = R$, the point $(0, 0, R)$ is singular, and the tangent space is two-dimensional.

4.1.2 The tangent space at a regular point

The following result states that at regular points, infinite dimensional manifolds have the same structure as finite dimensional ones.

Lemma 49 *Lyusternik)*
The tangent space *to $\mathcal{M}$ at a regular point $u \in \mathcal{M}$ is the set*

$$T_u\mathcal{M} := \{ \ v \in \mathcal{U}_0 \ \mid \ \delta\mathcal{K}_1(u; v) = \ldots = \delta\mathcal{K}_p(u; v) = 0 \ \}. \tag{4.2}$$

The result states that the tangent space consists of elements v that satisfy p linear constraints: it is a hyperplane in the function space, with finite codimension p (since the constraints are linearly independent).

A clearer geometric picture is obtained if we use the notation with the variational derivative. Then, at least for $\eta \in C_0^\infty \subset \mathcal{U}_0$,

$$\delta\mathcal{K}(u; \eta) \equiv \langle \delta\mathcal{K}(u), \eta \rangle,$$

and

$$T_u\mathcal{M} \supset \{ \ \eta \in C_0^\infty \subset \mathcal{U}_0 \ \mid \ \langle \delta\mathcal{K}_1(u), \eta \rangle = \ldots =< \delta\mathcal{K}_p(u), \eta >= 0 \ \}.$$

This makes it clear that the test functions from the tangent space satisfy p orthogonality conditions, namely orthogonal to the p normal directions $\delta\mathcal{K}_1, \ldots, \delta\mathcal{K}_p$: the tangent space is of co-dimension p.
We can use this (intuitive) interpretation in te proof of the Lemma, although the following examples motivate why we have to work with the linear functionals that are the first variations of the functionals, instead of with the variational derivatives only.

Exercise 50 Consider the set

$$\mathcal{M} = \{ \ u : [0, 1] \to \mathcal{R} \ \mid \ \mathcal{K}(u) = 1, u(0) = 1 \ \}.$$

1. For $\mathcal{K}(u) = \int \frac{1}{2} u^2$ the tangent space is

$$T_u\mathcal{M} = \{ \ v; [0, 1] \to \mathcal{R} \ \mid \ \int uv = 0, v(0) = 0 \ \},$$

   i.e. the functions with $v(0) = 0$ perpendicular to the variational derivative $\delta\mathcal{K}(u) = u$, just as is the case for test functions.

2. For $\mathcal{K}(u) = \int \frac{1}{2} u_x^2$ the tangent space is

$$T_u\mathcal{M} = \{\ v; [0,1] \to \mathcal{R}\ \mid\ \int u_x v_x = 0, v(0) = 0\ \};$$

relating this to the variational derivative $\delta\mathcal{K}(u) = -u_{xx}$ we find that v has to satisfy

$$\langle \delta\mathcal{K}(u), v\rangle + u_x(1)v(1) = 0, \text{ and } v(0) = 0.$$

So, for test functions η this means $\langle \delta\mathcal{K}(u), \eta\rangle = 0$, but there are more functions in the tangent space when $v(1) \neq 0$. These last functions should certainly be considered in the stationarity condition (the multiplier rule) in order to find the correct natural boundary conditions.

3. In more dimensions, an example of a nonlinear boundary condition is

$$\mathcal{M} = \{\ u : \Omega \to \mathcal{R}\ \mid\ u(x) = \varphi(x) \text{ on } \partial\Omega_1,\ \int_{\partial\Omega_2} u^2(x) = 1\ \}.$$

The tangent space is given by

$$T_u\mathcal{M} = \{\ v : \Omega \to \mathcal{R}\ \mid\ v(x) = 0 \text{ on } \partial\Omega_1,\ \int_{\partial\Omega_2} u(x)v(x) = 0\ \}$$

and clearly contains all test functions.

4.2 Lagrange's multiplier rule

4.2.1 Formulations

Recall the general stationarity condition (2.7) for a critical point $\hat{u}$ of $\mathcal{L}$ on $\mathcal{M}$:

$$\delta\mathcal{L}(\hat{u}; v) = 0, \text{ for all } v \in T_{\hat{u}}\mathcal{M}.$$

Using Lyusterniks Lemma for the specific set $\mathcal{M}$ under consideration, this condition for a critical point can be reformulated to

$$\begin{array}{lll} \delta\mathcal{L}(\hat{u}; v) = 0, & \text{for all} & v \in \mathcal{U}_0 \\ & \text{for which} & \delta\mathcal{K}_k(\hat{u}; v) = 0, 1 \leq k \leq p. \end{array} \tag{4.3}$$

In words: the null-space of the linear functional $\delta\mathcal{L}(\hat{u};\cdot)$ on $\mathcal{U}_0$ contains the intersection of the null spaces of the linear functionals $\delta\mathcal{K}_k(\hat{u};\cdot)$.
Clearly, (4.3) is satisfied if $\delta\mathcal{L}(\hat{u};\cdot)$ is a linear combination of the $\delta\mathcal{K}_k(\hat{u};\cdot)$, $1 \leq k \leq p$. In fact this is also necessary, as expressed in the next proposition.

Proposition 51 Lagrange's multiplier rule
A regular point $\hat{u} \in \mathcal{M}$ is a constrained critical point of $\mathcal{L}$ on $\mathcal{M}$, i.e. satisfies (4.3), if and only if there are real numbers, called Lagrange multiplier*s, $\lambda_1, \dots, \lambda_p$ such that*

$$\delta\mathcal{L}(\hat{u}; v) = \sum_k \lambda_k \delta\mathcal{K}_k(\hat{u}; v), \quad \textit{for all} \quad v \in \mathcal{U}_0. \tag{4.4}$$

It is possible to formulate this result in a different way; this may be easier to remember, but may also be somewhat misleading.

Proposition 52 *A regular point $\hat{u} \in \mathcal{M}$ is a critical point of $\mathcal{L}$ on the constrained set $\mathcal{M}$ (4.1) iff for some multipliers $\lambda_1, \dots, \lambda_p$ the element $\hat{u}$ is an* unconstrained *critical point of the* unconstrained *functional*

$$\mathcal{U} \ni u \mapsto \mathcal{L}(u) - \sum_m \lambda_m \mathcal{K}_m(u). \tag{4.5}$$

This functional is called the Lagrangian functional[1] *of the constrained problem.*

Proof. For a critical point of the Lagrangian functional it holds that

$$\delta[\mathcal{L} - \sum_m \lambda_m \mathcal{K}_m](u; v) = 0, \text{ for all } \ v \in \mathcal{U}_0.$$

This is precisely the equation from the multiplier rule. The other way around is obvious.

Warning. The above formulation with the Lagrangian may be misleading in the following respect: it may be possible that $\hat{u}$ is a constrained minimizer, while it is not a minimizer, but only a saddle point of the unconstrained Lagrangian; we will consider this in more detail later. On the other hand, this procedure does lead to the correct set of equations, including possible natural boundary conditions.

The results above have obvious consequences for the relation between the variational derivatives since $C_0^\infty \subset \mathcal{U}_0$. When no natural boundary conditions appear, these relations are in fact equivalent to the original result. The investigation of natural boundary conditions, in which the multipliers may appear, should be based on a study of (4.4).

Proposition 53 *For a constrained critical point $\hat{u} \in \mathcal{M}$ it holds that the variational derivatives are dependent:*

$$\delta\mathcal{L}(\hat{u}) = \sum_m \lambda_m \delta\mathcal{K}_m(\hat{u}).$$

Equivalently: the variational derivative of the Lagrangian functional vanishes. Possible natural boundary conditions are overlooked in this formulation.

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[1] Note that the name "Lagrangian" (functional) appears at various places with a different meaning!

4.2.2 Proof of the multiplier rule

4.3 Constrained Second Variation

For the manifold $\mathcal{M}$ given in (4.1) we calculate the second variation at a constrained critical point $\hat{u}$ that satisfies (4.4).
To that end, take $v \in T_{\hat{u}}\mathcal{M}$ and investigate for which functions w, depending on ε and v, the curve

$$\varepsilon \mapsto \hat{u} + \varepsilon v + w$$

belongs to $\mathcal{M}$, i.e. satisfies the constraints. Assuming $w = o(\varepsilon)$ from the start (i.e. $w/\varepsilon \mapsto 0$ for $\varepsilon \mapsto 0$), it follows from

$$\begin{aligned} \mathcal{K}(\hat{u} + \varepsilon v + w) &= \mathcal{K}(\hat{u}) + \delta\mathcal{K}(\hat{u}; \varepsilon v + w) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{K}(\hat{u}; v) + o(\varepsilon^2) \\ &= \mathcal{K}(\hat{u}) + \delta\mathcal{K}(\hat{u}; w) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{K}(\hat{u}; v) + o(\varepsilon^2) \end{aligned} \tag{4.6}$$

that w has to satisfy

$$\delta\mathcal{K}_k(\hat{u}; w) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{K}_k(\hat{u}; v) + o(\varepsilon^2) = 0, \tag{4.7}$$

for $1 \le k \le p$. Calculating the functional $\mathcal{L}$ on such a curve, using equation (4.4) for $\hat{u}$, produces

$$\begin{aligned} &\mathcal{L}(\hat{u} + \varepsilon v + w) \\ &\quad = \mathcal{L}(\hat{u}) + \varepsilon\delta\mathcal{L}(\hat{u}; v) + \delta\mathcal{L}(\hat{u}; w) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{L}(\hat{u}; v) + o(\varepsilon^2) \\ &\quad = \mathcal{L}(\hat{u}) + \sum_k \lambda_k \delta\mathcal{K}_k L(\hat{u}; w) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{L}(\hat{u}; v) + o(\varepsilon^2). \end{aligned} \tag{4.8}$$

Inserting the expression for $\delta\mathcal{K}_k(\hat{u}; w)$ from (4.7), there results:

$$\begin{aligned} &\mathcal{L}(\hat{u} + \varepsilon v + w) = \\ &\qquad \mathcal{L}(\hat{u}) + \frac{1}{2}\varepsilon^2 \left[\delta^2\mathcal{L}(\hat{u}; v) - \sum_k \lambda_k \delta^2\mathcal{K}_k(\hat{u}; v)\right] + o(\varepsilon^2) \end{aligned} \tag{4.9}$$

The expression

$$\delta^2\mathcal{L}(\hat{u}; v) - \sum_k \lambda_k \delta^2\mathcal{K}_k(\hat{u}; v) \tag{4.10}$$

for $v \in T_u\mathcal{M}$ is called the *constrained second variation* of $\mathcal{L}$ on the manifold $\mathcal{M}$ at the critical point $\hat{u}$. Note that it is precisely the (unconstrained) variation of the Lagrangian functional (4.5) that leads to the equation for $\hat{u}$, but restricted to variations form the tangent space.

Proposition 54 *If $\bar{u}$ is a local extremal for $\mathcal{L}$ on the manifold $\mathcal{M}$ given by (4.1), that satisfies the multiplier equation (4.4), the constrained second variation (4.10) is sign-definite in all directions v from the tangent space.*
Specifically, if $\mathcal{L}$ has a (local) minimum at $\bar{u}$, then

$$\delta^2\mathcal{L}(\bar{u};v) - \sum_k \lambda_k \delta^2\mathcal{K}_k(\bar{u};v) \geq 0 \textit{ for all } v \in T_{\bar{u}}\mathcal{M}. \tag{4.11}$$

4.4 Families of constrained problems

Although the following can be formulated in a much more general way, we restict to illustrate the general ideas to a simple example: the constrained optimization of one functional H on level sets of another functional I:

$$\text{Crit } \{H(u) \mid I(u) = \gamma\};$$

we will use the formulation with variational derivatives in the following, not bothering about possible natural boundary conditions.

In the previous sections we studied the problem with fixed value of the constraint, i.e. given γ. Now we will treat γ as a parameter, and consider the family of constrained optimization problems. This will enable us to give an interpretation of the multiplier and relate the nature of the constrained critical point to its character as a critical point of the Lagrangian functional.

Suppose therefore that we can find a smooth family

$$\gamma \mapsto U(\gamma) \in \text{Crit } \{H(u) \mid I(u) = \gamma\}$$

of constrained critical points of H on level sets $I^{-1}(\gamma)$ for parameter values γ in a neighbourhood of some γ_0. It may happen that, for instance, this family consists only of constrained minimizers, but also that the character of the critical point changes with γ (without violating the smoothness assumption).

A first observation is that the derivative along this family is "normal" to the level sets of I in the following sense. Defining

$$n(U) := \frac{dU}{d\gamma}, \tag{4.12}$$

it is found by differentiating the relation $I(U(\gamma)) = \gamma$ with respect to γ, that $n(U)$ is normal to the level set $I^{-1}(\gamma)$ in the sense that

$$\langle \delta I(U), n(U) \rangle = 1. \tag{4.13}$$

Along this branch, each element satisfies for a multiplier $\lambda = \lambda(\gamma)$ the equation

$$\delta H(U(\gamma)) = \lambda(\gamma)\delta I(U(\gamma)). \tag{4.14}$$

The multiplier can be related to the so-called value function.

Definition 55 *The* value function *of the constrained critical point problem on a branch of critical points is defined as:*

$$h(\gamma) := H(U(\gamma)) = Crit\ \{H(u) \mid I(u) = \gamma\}. \tag{4.15}$$

The value function can be depicted in a so-called *integral diagram*. With the value of the integrals H and I along the axis, each point represents all states with that value of H and I (a two-dimensional representation of the state space). Assuming that there are branches of constrained critical points parameterized with the value of the constraint functional γ, a schematic representation of these equilibria in the integral diagram may look like Fig. 4.1.

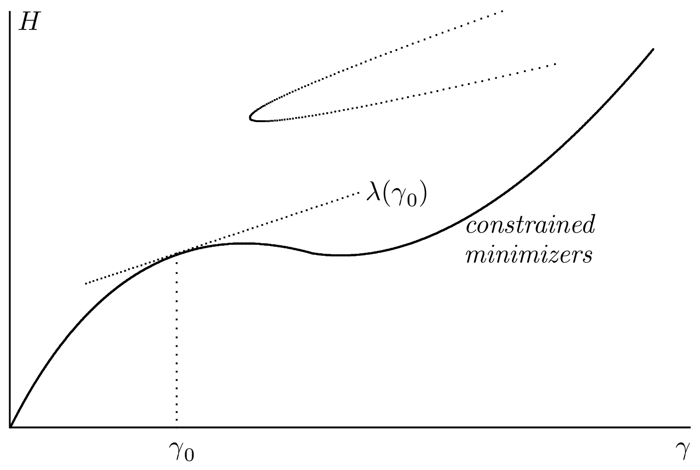

Figure 4.1: The integral diagram. Schematic presentation of the value function of the constrained minimization problem (solid line). No states correspond to points below this solid line. The tangent to this curve has slope $\lambda(\gamma)$. Other curves (dotted) represent branches of relative equilibria that correspond to different families of constrained critical points such as local minimizers, saddle points, and (local) maximizers.

Both the first and second derivative of the value function play a particular role in the understanding of the critical point problem; this will be considered in the nect two subsections.

4.4.1 The multiplier as derivative of the value function

Proposition 56 *For the smooth family $\gamma \mapsto U(\gamma)$, the multiplier $\lambda(\gamma)$ appearing in (4.14) is related to the value function according to*

$$\lambda(\gamma) = \frac{dh(\gamma)}{d\gamma}. \tag{4.16}$$

Proof. A direct differentiation with respect to γ leads to the result:

$$\frac{dh(\gamma)}{d\gamma} = \langle \delta H(U(\gamma)), \frac{dU(\gamma)}{d\gamma} \rangle = \lambda \langle \delta I(U(\gamma)), n(U) \rangle = \lambda,$$

the last equality from differentiation of $I(U(\gamma)) = \gamma$.
This result clearly shows that only by viewing a single problem for γ_0 as being embedded in a family provides an interpretation of the Lagrange multiplier $\lambda(\gamma_0)$.

4.4.2 Constrained minimizers as critical points of the Lagrangian functional

The character of the constrained critical point at γ_0 can be related to its character as a critical point of $u \mapsto H(u) - \lambda(\gamma_0) I(u)$. This is determined by the second derivative.

Proposition 57 *The second variation of the constrained problem in the normal direction $n(U)$ defined in (4.12), is precisely the second derivative of the value function:*

$$\langle [D^2 H(U) - \lambda D^2 I(U)] n(U), n(U) \rangle = \frac{d^2 h(\gamma)}{d\gamma^2}. \tag{4.17}$$

In particular it follows that the sign *of the second variation in this direction is determined by the* convexity *or* concavity *of the value function in a neighbourhood of the value of γ.*

Proof. Differentiating the equation (4.14) with respect to γ there results

$$[D^2 H(U) - \lambda D^2 I(U)] n(U) = \frac{d\lambda}{d\gamma} \delta I(U). \tag{4.18}$$

Since $d\lambda / d\gamma = d^2 h(\gamma) / d\gamma^2$, (4.17) results after taking the inner product with $n(U)$.

In the foregoing Propositions, U can also be viewed as a critical point of the Lagrangian functional $H - \lambda I$ on the whole space. The expression (4.17) gives information how this functional changes in the direction transversal to level sets of I. This may determine the character of U as an unconstrained critical point of $H - \lambda I$.

Proposition 58 *A constrained minimizer of H on level set of I is an unconstrained (local) minimizer of $H - \lambda I$ (where λ is the multiplier) if the value function is (locally) convex. If the value function is (locally) concave, a constrained minimizer is an unconstrained saddle point of $H - \lambda I$.*

Proof. It would be tempting to use the second variation to provide the proof. Indeed, being constrained minimal, the second variation is non-negative on the tangent space, and the previous result shows the sign in the remaining direction transversal (normal) to the tangent space. This is correct if certain technical conditions are met, viz. non-degeneracy (signs strictly positive or negative), and a property that sign-definiteness of the second variation is sufficient for minimality. However, the following reasoning is elegant and simple, and does not need any of such requirements.
Let U_0 be a constrained minimizer of H on the level set $I = \gamma_0$, with λ_0 the multiplier. Assuming that the value function is (locally) convex (i.e. $d^2h(\gamma)/d\gamma^2(\gamma_0) > 0$), the result that U_0 is in fact an unconstrained (local) minimizer of the functional $H - \lambda_0 I$ follows by comparing its value with arbitrary functions u, with $I(u) = \gamma$, γ in a neighbourhood of γ_0:

$$\begin{aligned}
&H(u) - \lambda_0 I(u) \\
&\quad \geq \; h(\gamma) - \lambda_0 \gamma \text{ by definition of } h \\
&\quad \geq \; h(\gamma_0) - \lambda_0 \gamma_0 \text{ from convexity of } h \\
&\quad = \; H(U_0) - \lambda_0 I(U_0) \text{ since } U_0 \text{ is a constrained minimiser.}
\end{aligned}$$

If h is locally concave, $H - \lambda_0 I$ is maximal on the family $\gamma \mapsto U(\gamma)$, and the saddle point character is clear. See Fig. 4.2.

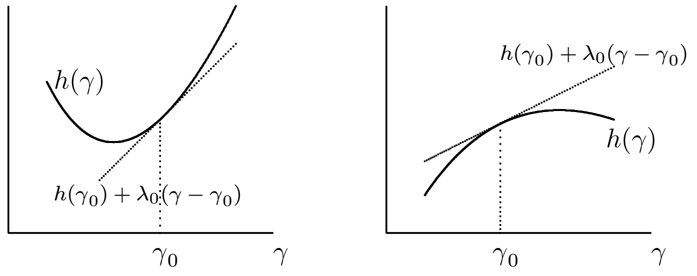

Figure 4.2: With the bold line the graph of the value function h, the tangent to this graph at $\gamma_0 : \gamma \mapsto h(\gamma_0) + \lambda_0(\gamma - \gamma_0)$, lies below this graph if h is locally convex (at the left), or above this graph if h is locally concave (at the right). In the convex case, a constrained minimizer is actually an unconstrained minimizer of the functional $H - \lambda_0 I$; in the concave case a constrained minimizer is a saddle point of $H - \lambda_0 I$.

4.5 Exercises

1. *Lemma DuBois-Reymond, integrated Euler-Lagrange equation*
   We start with a generalization of Lagrange's Lemma, and then show how

it can be used to weaken the regularity assumptions for a critical point that were required in the first chapter.

(a) Use the (linear) multiplier rule to prove the following

Proposition 59 Lemma DuBois-Reymond
Let $f \in C^0([0,1])$ *satisfy*

$$\langle f(x), \xi(x) \rangle = 0, \text{ for all } \xi \in C_0^\infty \text{ with } \int_0^1 \xi(x)dx = 0.$$

Then f *is constant on* $[0,1]$.

(b) Give a different proof (based on Lagrange's Lemma) by reformulating the information for f by observing that

$$\{\eta_x \mid \eta \in C_0^\infty([0,1])\} \equiv \{\xi \in C_0^\infty([0,1]) \mid \int_0^1 \xi(x)dx = 0\}.$$

Observe that this method requires the assumption that f is differentiable!

(c) An extension of the foregoing is immediate:
Let $f \in C^0([0,1])$ *satisfy*

$$\langle f, \eta_{xx} \rangle = 0 \text{ for all } \eta \in C_0^\infty([0,1]).$$

Then f *is a linear function on* $[0,1]$.
Provide the proof, first by assuming $f \in C^2$ and using Lagrange's Lemma, then without additional smoothness assumptions on f by observing

$$\{\eta_{xx} \mid \eta \in C_0^\infty([0,1])\} \equiv \{\xi \in C_0^\infty([0,1]) \mid \int_0^1 \xi(x)dx = \int_0^1 x\xi(x)dx = 0\}.$$

(d) *Integrated Euler-Lagrange equation for single integral problems*
For the single integral functional $\mathcal{L}(u) \equiv \int_a^b L(u, u_x)dx$, and the expression for the first variation

$$\delta\mathcal{L}(u;\eta) = \int [L_u \eta + L_{u_x} \eta_x] dx$$

the Euler-Lagrange equation was found in Chapter 1 by partial integration of the last term. This required the assumption that L_{u_x} is differentiable, which ususally requires the assumption that $u \in C^2$. Show that, by partial integration of the first (!) term, this assumption can be avoided when using the results of the Lemma of DuBois-Reymond above. The result is then the integrated form of the Euler-Lagrange equation:

$$-\int^x [L_u] + L_{u_x} = \text{ constant on } [a,b].$$

Inspecting this integrated form, conclude that at a critical point $\hat{u} \in C^1$ actually L_{u_x} is differentiable. In most cases this implies that actually $\hat{u} \in C^2$. This means that for a critical point *additional regularity is obtained from the stationarity condition!*
Illustrate this to the simple case $L = \frac{1}{2}u_x^2 - V(u)$.

2. *Linear boundary conditions as constraints*
   In this exercise we show that linear boundary conditions can also be treated as constraints from the start on, a somewhat different approach as taken in the theory of this chapter.

   (a) Consider in a linear space $\mathcal{U}$ of functions defined on Ω the set $\mathcal{M}$ described with linear boundary functionals

   $$\mathcal{M} = \{\ u \ \mid\ \ell(u) = c\ \},$$

   where ℓ is a boundary functional. Show that for a critical point $\hat{u}$ of a density functional $\mathcal{L}$ on $\mathcal{M}$ it holds that

   $$\delta\mathcal{L}(\hat{u}; v) = 0, \text{ for all } v \in \mathcal{U} \text{ with } \ell(v) = 0.$$

   (b) Let $\mathcal{B}(\hat{u}; v)$ be the boundary functional that appears when writing the first variation with the variational derivative like

   $$\delta\mathcal{L}(\hat{u}; v) = \langle \delta\mathcal{L}(\hat{u}), v\rangle + \mathcal{B}(\hat{u}; v).$$

   Conclude that on the boundary it should hold that

   $$\mathcal{B}(\hat{u}; v) = 0, \text{ for all } v \in \mathcal{U} \text{ with } \ell(v) = 0.$$

   (c) Use the multiplier rule (for the boundary functionals) to conclude that for some multiplier

   $$\mathcal{B}(\hat{u}; v) = \lambda\ell(v), \text{ for all } v \in \mathcal{U}.$$

   (d) Show that this is the same result as would be obtained when investigating

   $$\text{Crit } \{\mathcal{L}(u) \mid \ell(u) = c\},$$

   for which the result is that there exist a multiplier λ such that it is also a solution of the unconstrained Lagrangian functional

   $$\text{Crit } \{\mathcal{L}(u) - \lambda\ell(u) \mid u \in \mathcal{U}\}.$$

   (e) Use the method above to treat the following problems

   $$\text{Crit}_{u(x_0)=u_0} \int_{x_0}^{x_1} L(x, u, u_x),$$

   $$\text{Crit } \left\{ \int_\Omega \{\frac{1}{2}|\nabla u|^2 - f(x)u\}dx \mid u(x) = \phi(x) \text{ on } \partial\Omega_1 \right\}.$$

3. Prove Lagrange's Multiplier Rule for the case of one constraint.

4. Consider for $\gamma > 0$ the value function of the minimization problem

$$h(\gamma) = \text{Min}\ \left\{ \int_0^\pi \left[u_x^2 + u^2\right] dx \;\middle|\; \int_0^\pi u^4 dx = \gamma, u(0) = u(\pi) = 0 \right\}.$$

Determine, up to a multiplicative factor, the value function by using the homogeneity of the functionals (do not try to calculate the minimizers explicitly).

Chapter 5

Variational structures in Science II

5.1 Geometric problems

Following are a few of the classical problems that deal with constrained problems. (Exploit "energy conservation" to help to solve the equations explicitly.)

Exercise 60

1. *Dido's problem*
   Find the surface of largest area, given the value of its perimeter.
2. *Chain line*
   Find (from minimal potential energy) the form of a chain with prescribed length hanging in the (constant) gravitational field between given points.
3. *Brachistochrone*
   Determine the shape of a curve of given length in the vertical plane that is such that the time for a particle (starting with zero initial velocity at the highest end point) to reach the other point is as small as possible (friction neglected).

5.2 Constrained minimal energy: Relative Equilibria

In this section we briefly describe the main ideas and some examples how constrained problems appear in dynamical systems. Later a more extensive treatment is given.

Recall that for an autonomous Hamiltonian system the energy (Hamiltonian) H is conserved. Critical points of H are equilibria for the dynamics.

When there is an additional first integral, say I, it turns out that there is a natural way to "unfold" the equilibria into so-called *relative equilibria*. Before showing the relevance for the dynamics, the idea is simply as follows.
When looking for a minimizer (it also holds for other critical points) of H, one compares the value of H with the value at *all* other possible states.
When an additional integral I exists, any dynamical evolution remains on a level set of I. The unconstrained minimization compares states at different level sets of I. By restricting to a minimum energy state at an a priori given level set of I one is led to consider the constrained optimization problem

$$\text{Min } \{H(u) \mid I(u) = \gamma\}.$$

This is clearly an example of the unfolding of the minimizers of H, i.e. of the equilibria of the Hamiltonian system. It turns out that the constrained critical points form a set that is invariant for the dynamics. Even more so, the constrained critical points found in this way are called relative equilibria: there is a dynamic evolution, but a very specific one, in this invariant set. So, also in this dynamic respect, the relative equilibria are a true generalization of the equilibria.

In many applications from Mathematical Physics, the constrained energy minimizers are *coherent structures*, like solitons in the theory of surface waves or electro-magnetic pulse propagation in glass-fibres, vortices in plane fluids, etc. Taking such a state as initial data, the dynamcs is then simply a translation or rotation with uniform velocity: simple dynamical evolutions compared to the often terribly complicated dynamics of an arbitrary initial data.
The general theory (for Poisson systems) will be treated later(see also Van Groesen & De Jager); here we treat a specific case (for Hamiltonian systems) in a nut shell.

1. *Hamiltonian flows*
   Write a Hamiltonian system like

   $$\partial_t u = J\delta H(u).$$

   For a finite dimensional, canonical, system, $u = (q,p) \in \mathcal{R}^{2N}$, $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ the symplectic matrix, and $\delta H(u) = \nabla H = \begin{pmatrix} \partial_q H \\ \partial_p H \end{pmatrix}$.
   Denote the solution with initial value u_0 with the so-called H-flow as

   $$u(t) = \Phi_t^H(u_0),$$

   indicating the dependence on H and on the initial value. Determine for instance the flow for $H = \frac{1}{2}(p^2 + \omega^2 q^2)$. Observe that

   $$\partial_t \Phi_t^H(u_0)\big|_{t=0} = J\nabla H(u_0)$$

2. *Invariance of H for the I-flow*

(a) Write down the condition that I is a first integral.

(b) Show that the constancy of I means that

$$I(\Phi_t^H(u_0)) = I(u_0), \text{ for all } t$$

Differentiate this identity with respect to the initial condition and with respect to t (and then take $t = 0$) to find that

$$-H''(u_0)J\delta I(u_0) = \delta I(u_0) \quad \text{for all } u_0.$$

Verify that in the same way it holds that

$$-I''(u_0)J\delta H(u_0) = \delta H(u_0) \ \text{ for all } u_0.$$

3. *Relative equilibrium solutions*
Let U be a relative equilibrium, i.e.

$$U \in \text{Min } \{H(u) \mid I(u) = \gamma\}.$$

(a) Observe that with U also $U(\phi) \equiv \Phi_\phi^I U$ is a solution for all ϕ. Hence the relative equilibria come in branches: the minimization problem is degenerate. Show that all these minimizers satisfy the same equation $\delta H(U(\phi)) = \lambda \delta I(U(\phi))$ (all with the same multiplier).

(b) Verify by direct substitution into the dynamic equation that the function

$$t \mapsto U(\lambda t)$$

is a dynamic solution, the so-called *relative equilibrium solution.*

Exercise 61 *1.* Derive the equation for spherical pendulum using as Lagrangian the difference of kinetic and potential energy, expressed in spherical angle coordinates.

2. Show that the dynamics is a Hamiltonian system with Hamiltonian

$$H = \frac{1}{2}\left(p_\theta^2 + \frac{p_\phi^2}{\sin^2\theta}\right) + \omega_0^2(1 - \cos\theta)$$

3. Observe that there is, except from H, an additional first integral I, the socalled angular momentum.

4. Reduce the dynamics by prescribing the value of I, and find equilibria of this reduced dynamics.

5. Show that the equilibria of the reduced dynamics are in fact the relative equilibria: constrained minimizers of H at given I.

6. Determine the relative equilibrium solutions and interpret their motion in space. Relate the angular velocity to (the derivative) of the relevant value function.

Exercise 62 The KdV (Korteweg - de Vries, 1895) equation has been derived to describe the motion of surface waves on a layer of fluid above an horizontal bottom. For the wave elevation $u(x,t)$ the equation (in normalized form) reads

$$\partial_t u = -\partial_x (u_{xx} + 3u^2).$$

The equation will be considered on the whole real line (solutions decaying sufficiently fast to zero, together with their derivatives).

1. Show that the equation can be rewritten like

$$\partial_t u = \partial_x \delta H(u)$$

for the Hamiltonian (normalized energy)

$$H(u) = \int (\frac{1}{2} u_x^2 - u^3).$$

This is of the form of a continuous Hamiltonian system, with the symplectic matrix replaced by the differential operator ∂_x. Show that the Hamiltonian is conserved as a consequence of the skew-symmetry of ∂_x.

2. A *travelling wave* is a solution of the form

$$t \mapsto U(x - \lambda t);$$

here U is the waves shape and λ the speed of propagation. Derive the o.de. for U in order that the KdV equation is satisfied.

3. Show (phase plane analysis) that there exist a unique positive solution for any value of $\lambda > 0$. To that end, first observe that the o.de. itself can be written as a second order Hamiltonian system with the spatial variable as the "time"; determine the potential energy (depending on λ) and draw level-lines of the "total energy".
Obsere that the solution sought for (i.e. satisfying the decaying conditions at infinity) is the homoclinic orbit in this phase diagram.
Investigating the formula for U, derive an explicit expression for U. This solution is the so-called soliton solution of KdV.

4. Verify that the following functional is a first integral, different from the Hamiltonian, for the p.de.:

$$I(u) = \int \frac{1}{2} u^2.$$

This is a momentum-type of integral: its flow is translation, and its constancy for KdV is a consequence of the translation symmetry of the KdV-Hamiltonian.

5. Write down the equation for the relative equilibria for H on levelsets of I; compare this with the equation for travelling waves.

6. Determine the relative equilibrium solution.

Remark 63 In optimization problems that arise from dynamics, as in the examples above, the process of *unfolding* has various important physical aspects. When the problem has several first integrals, all the relative equilibria have a specific dynamic evolution, the so-called relative equilibrium solution. When more integrals are available, by constructing constrained energy extremizers with more integrals, more difficult relative equilibria are obtained, depending on more variables. Those solutions are ususally very interesting for the dynamics. In the sense defined above, they can be seen as an unfolding obtained from simpler relative equilibria by adding constraints. The reverse process of unfolding, *defolding*, sometimes takes place in dynamic systems, and is then referred to as self-organization. For instance, in dissipative systems, selective dissipation of integrals may lead to this reversed process: self-organization to simpler states, for instance from an initial state in $\mathrm{MRE}(H, I_1, I_2)$ (where MRE denotes "Manifold of Relative Equilibria") to an intermediate state in $\mathrm{MRE}(H, I_1)$ to an equilibrium in $\mathrm{E}(H)$.
It should also be noted that in many dynamic problems, the unfolding is degenerate, and so the process when viewed from the equation, is non-smooth (multipliers that are not smoothly changing with the constraints).

5.3 Thermodynamic systems

We have seen that gradient systems can be used for numerical purposes to find the minimizer of a given functional; the dynamic trajectories are in the direction of steepest descent.

When looking for constrained minimizers, this method has to adapted to take the constraints into account. We briefly describe the modification; for simplicity we restrict ourselves to the case of one functional constraint.
These systems are called thermodynamic systems, since there is one integral that is conserved (the "energy") while another one decreases monotonically (the "entropy")[1].

Definition 64 *A* thermodynamic system *is a dynamical system in the state space $\mathcal{U}$ that is of the form*

$$\partial_t u = -[\delta H(u) - \lambda(u)\delta I(u)], \quad \textit{with } \lambda(u) = \frac{\langle \delta I(u), \delta H(u)\rangle}{\langle \delta I(u), \delta I(u)\rangle}$$

where $H : \mathcal{U} \to \mathcal{R}$ and $I : \mathcal{U} \to \mathcal{R}$ are functionals.

---

[1] From a mathematical point of view, the system can also be considered as a simple example of a dynamical system on a manifold: the level set of the conserved functional as the manifold on which a disspative system is defined.

To see the dynamic properties, observe that any functional F evolves according to

$$\partial_t F(u) = \langle \delta F(u), [\delta H(u) - \lambda(u)\delta I(u)]\rangle.$$

Substituting the functional I for F and the expression for $\lambda(u)$, it follows that

$$\partial_t I(u) = \langle \delta I(u), [\delta H(u) - \lambda(u)\delta I(u)]\rangle = 0$$

Hence, for the dynamics the functional I is conserved, a constant of the motion, a *first integral*:

$$I(u(t)) = I(u(0)) \text{ for all } t.$$

Geometrically this is seen since the vectorfield $\delta H - \lambda\delta I$ is perpendicular to δI, and so tangent to the level sets of I.

On each level set of I, the system behaves like a dissipative system as treated in the foregoing chapter. In fact, for the evolution of H:

$$\begin{aligned}\partial_t H(u) &= \langle \delta H(u), [\delta H(u) - \lambda(u)\delta I(u)]\rangle \\ &= \langle [\delta H(u) - \lambda(u)\delta I(u)], [\delta H(u) - \lambda(u)\delta I(u)]\rangle,\end{aligned}$$

so

$$\partial_t H(u) \begin{cases} \leq 0 \\ = 0 \text{ iff } \delta H(u) = \lambda \delta I(u) \end{cases}.$$

From this it follows that H decreases monotonically, except from the points that are the equilibria of the system. Indeed, an equilibrium solution satisfies the equation

$$\delta H(\hat{u}) = \lambda \delta I(\hat{u})$$

for some scalar λ. Recalling Lagrange's multiplier rule, this is the equation for constrained critical points of H on a level set of I:

$$\hat{u} \in \text{Crit } \{H(u) \mid I(u) = \gamma\}.$$

From the above observations it is clear that the trajectories are in the direction of *constrained steepest descent*; hence the equation can be used to find constrained minimizers of H on level sets of I in a numerical way.

Exercise 65 *1.* The dynamic system above provides a way to prove Lagrange's multiplier rule in an alternative way, different from the proof as given before. Give the detailed argumentation.

2. Write down the equation of constrained steepest descent to find the solution of

$$Min \ \{\int u_x^2 \mid \int u^2 = 1, u(0) = u(\pi) = 0\},$$

and investigate the convergence to the minimal element.

5.4 Exercises

1. *Periodic oscillations of constrained (pseudo-) potential energy*
   When looking for periodic solutions of a second order system with potential energy V

   $$-\ddot{q} \; = \; V'(q), \quad q(0) = q(T), \; \dot{q}(0) = \dot{q}(T),$$

   where the period T is not prescribed in advance, one may try to use the constrained critical point problem

   $$\begin{aligned} \text{Crit } \{\mathcal{K}(x) \mid \mathcal{V}(x) \; &= \; R, x \in X\}, \\ \text{with } \mathcal{K}(x) \; &= \; \int_0^1 \frac{1}{2}|\dot{x}|^2 d\tau, \;\; \mathcal{V}(x) = \int_0^1 V(x) d\tau \end{aligned}$$

   and $X = \{ \; x \in C^1([0,1]) \;\mid\; x(0) = x(1) \; \}$.

   (a) Give sufficient conditions for the potential energy function $\mathcal{V}$ that imply that the multiplier in the equation for the constrained critical points:

   $$-\ddot{x} = \lambda V'(x)$$

   is positive.

   (b) Show that, when $\lambda > 0$, the critical points $x(\tau)$ correspond to the desired periodic solutions up to a scaling of the time variable. Give the physical meaning of the functionals $\mathcal{K}$ and $\mathcal{V}$ expressed in terms of $q(t)$.

   (c) The minimization problem Min $\{\mathcal{K}(x) \mid \mathcal{V}(x) = R, x \in X\}$ (assuming the constrained set to be non-empty) has a trivial solution, viz. a constant. Therefore, we have to look for non-minimal critical points.

   (d) One case in which non-trivial critical points can be found is when $\mathcal{V}$ is an even function: $\mathcal{V}(x) = \mathcal{V}(-x)$. Show that in that case periodic solutions can be found on an interval $[-1,1]$ by odd continuation of a critical point on $[0,1]$ of

   $$\text{Min } \{\mathcal{K}(x) | \mathcal{V}(x) = R, x \in X, x(0) = x(1) = 0\}.$$

   (e) Find the solutions when $x = (x_1, x_2)$ and $V(x) = x_1^2 + 3x_2^2$.

2. *Free fluid surface in a container*
   Consider a cylinder with axis vertically (in the direction of gravitation, the z-axis), partly filled with fluid. Assuming that the bottom of the cylinder is described at $z = 0$ by the region $\Omega \in \mathcal{R}^2$, the fluid surface will be described by $u = u(x,y)$, so that the fluid occupies the region

   $$\{ \; (x,y,z) \;\mid\; (x,y) \in \Omega, \; 0 \leq z \leq u(x,y) \; \}.$$

We are looking for the form of the free surface of the fluid, i.e. the function u, from a minimal energy principle when effects of surface tension and adhesion are taken into account.
To that end, let

- $S =$ the area of the free surface,
- $S^* =$ the area of the wetted part of the cylinder wall,
- $V =$ the volume of the water.

(a) Describe S, S^*, V as functionals of u.

(b) For given $V_0 > 0$ and $\sigma \in \mathcal{R}$ with $|\sigma| < 1$ the minimization problem

$$\text{Min } \{S(u) - \sigma S^*(u) | u \in C^1(\Omega), V(u) = V_0\}.$$

Interpret this optimization problem in physical terms as a minimum energy principle.

(c) Supposing that $\hat{u} \in C^2$, determine the governing boundary value problem for a minimizer $\hat{u}$.

(d) Write $\sigma = \sin\beta$, with $\beta \in (-\pi/2, \pi/2)$. Give the meaning of β. Sketch the form of the free surface for the two different cases that $\sigma < 0$ and $\sigma > 0$. (Can you give examples of fluids with these properties?)

(e) Express the multiplier that appears in the equation for $\hat{u}$ in terms of known quantities (σ, area of Ω, length of $\partial\Omega$).

(f) Approximate the functional S for surfaces for which ∇u is small, by a constant plus a quadratic functional $\bar{S}(u)$. Write down the governing boundary value problem.

(g) Consider the special case of a circular cylinder: $\partial\Omega$ is the circle with radius R. Introduce cylinder coordinates (r, ϕ, z) and write $\bar{S}, S^*, V$ as functionals of $u = u(r, \phi)$. Express the multiplier in terms of σ and R.
Determine explicitly the free surface for given σ and V_0 (sufficiently large) in the approximation considered.

(h) Find a lower bound for V_0 (given σ and R) for which a C^2-solution can be expected. What is the physical interpretation?

3. *Kink solutions of Sine-Gordon equation*
The Sine-Gordon equation describes with an angle variable the orientation of spins on a continuous line in an magnetic system. The equation reads (with κ some material constant)

$$u_{tt} = u_{xx} + \kappa \sin 2u.$$

(a) Derive the equation for a travelling wave: $u(x, t) = U(x - \lambda t)$.

(b) Show that there is a *kink-solution*, a travelling wave with $U(\xi) \to 0$ for $\xi \to -\infty$, and $U(\xi) \to \pi$ for $\xi \to \infty$; use phase plane analysis.

(c) Investigate the variational formulation for the kink solution.

4. *Cnoidal waves for KdV*

Travelling waves of KdV were investigated on the whole real line before. In this exercise we want to investigate travelling waves that are periodic.

(a) Show that solutions that are periodic with period 2π on the real line can be found by periodic continuation of functions on $[0, 2\pi]$ that satisfy periodic boundary conditions.

(b) Show that for periodic solutions it is possible to restrict to solutions with zero mass: $\int u = 0$.

(c) Derive the equation for a periodic travelling wave; investigate this equation (phase plane analysis). Derive the solution in an implicit way. Using elliptic functions, the so-called cnoidal function, the solution can be "explicitly" written down; therefore such periodic waves are called *cnoidal waves*.

(d) Show that the cnoidal wave *form* is obtained as a relative equilibrium form the constrained minimal energy problem

$$\text{Min} \int (\frac{1}{2}u_x^2 - u^3) \mid \int \frac{1}{2}u^2 = \gamma, \int u = 0, u(0) = u(2\pi),$$

and that the cnoidal wave is the corresponding relative equilibrium *solution.*

(e) In the rest of this exercise we study the constrained minimization problem; denote a solution by U (suppressing the dependence on γ that does not play a particular role in this exercise).

(f) Show that $u \equiv 0$ is a critical point, but not the minimizer.

(g) Conclude that for the minimizer $\int U^3 > 0$, and that U cannot be a constant.

(h) Observe that with U, any translate of U is also a minimizer: there is a continuum of minimizers.

(i) Construct the Lagrangian functional; show that this Lagrangian functional is not bounded from below. Hence, U is not the (global) minimizer of the Lagrangian functional.

(j) Now show that U is also not a local minimizer of the Lagrangian functional. To that end, investigate the second variation at U. First show that the second variation at U vanishes in the direction U_x (why?). Then show that the second variation at U in the direction U is negative (use the equation for U; note that the U-direction is not tangent to the level set of the constraint-functional!).

(k) Conclude from the previous result that the value function must be a concave function.

Chapter 6

Linear Eigenvalue Problems

Recall the linear eigenvalue problem from Linear Algebra:

> *Given a matrix A in R^n, find the values $\lambda \in C$, called eigenvalues, such that there exists a non-trivial vector x, called eigenvector, that satisfies*
>
> $$Ax = \lambda x.$$

In general, the eigenvalues are complex-valued; they are the solutions of the characteristic polynomial

$$det[A - \lambda Id] = 0.$$

A solution λ_p of this algebraic equation with *algebraic multiplicity* α_p defines at least one eigenvector; the number of independent eigenvectors is called the *geometric multiplicity* $\gamma_p (\leq \alpha_p)$. The difference $\alpha_p - \gamma_p$ determines the number of generalized eigenvectors.Hence, the set of eigenvectors does not define a complete set in $\mathcal{R}^n$ unless $\alpha_p = \gamma_p$ for all eigenvalues.
For matrices A that are symmetric, the situation is essentially simpler:

> *All the eigenvalues of a symmetric matrix S in R^n are real, and the eigenvectors form a complete set of vectors in R^n; with respect to this basis, the matrix S is in diagonal form*
>
> $$S \backsimeq diag\{\lambda_1, \ldots, \lambda_n\}$$
>
> *where $\lambda_1, \ldots, \lambda_n$ are the real eigenvalues (not necessarily different).*

In standard courses Linear Algebra, mosttimes the most general result is proved, and then the result for symmetric matrices is derived as a special consequence. When generalizing the results to linear operators in infinite dimensional spaces, the general result (spectral theory) turns out to be quite complicated, related to possible unboundedness of the operators. On the other hand, exploiting variational methods that can be used for symmetric operators, the special result

can be obtained much simpler in a more direct way. This will be the approach taken in this chapter[1]. After generalizing the notion of “symmetry" to linear operators, the eigenvectors will be obtained as critical points of the Rayleigh quotient; its value will be the eigenvalue. The principal eigenvalue will correspond to a minimizer (for differential operators) or to a maximizer (for integral operators). Other eigenvectors and eigenvalues will be found in a successive way by restricting the original space, exploiting the notion of natural constraint.
For comparioson arguments, and numerical procedures to calulate non-principal eigenvectors and eigenvalues, non-successive characterizations are very usefull, and will be considered also.

6.1 Formulation, examples

6.1.1 Linear operators in function spaces

Let X and Y be linear spaces, and $L : X \to Y$ a linear mapping (operator). In all our problems X, Y will be function spaces.
The eigenvalue problem for L asks for the eigenvalues λ that are the complex numbers for which there exists a non-trivial *eigenfunction* u:

$$Lu = \lambda u.$$

Clearly, since the domain of definition of L is X, and its range is Y, the eigenfunctions will be elements from the intersection $X \cap Y$ (which must be non-empty to allow eigenfunctions to exist at all).
To define the notion of a symmetric operator, we exploit (as in the previous chapters) the L_2-inner product for functions on the domain Ω.

Definition 66 *Let L be an operator between function spaces $\mathcal{U}$ and $\mathcal{V}$, both of which contain the test functions. Denote by $\mathcal{U}^*, \mathcal{V}^*$ the dual spaces of $\mathcal{U}, \mathcal{V}$ with respect to the L_2-innerproduct. The* formal adjoint *of L is the (linear) operator denoted by $L^* : \mathcal{V}^* \to \mathcal{U}^*$ such that*

$$\langle Lu, v^* \rangle =< u, L^* v^* > \text{ for all } u, v^* \in C_0^\infty(\Omega).$$

The operator L is called (formally) symmetric *on $\mathcal{U}$ if $L = L^*$ and moreover*

$$\langle Lu, v \rangle = \langle u, Lv \rangle \text{ for all } u \in \mathcal{U}.$$

Associated to L there is a bilinear functional

$$b(u, v) :=< Lu, v > .$$

---

[1] In this chapter we will concentrate on the theory for infinite dimensonal spaces. It should be noted that the method also provides the result stated above for symmetric matrices in $\mathcal{R}^n$; this gives a direct proof of the results without referring to the more general result for arbitrary matrices.

If L is (formally) symmetric on $\mathcal{U}$, this bilinear functional is symmetric and defines the quadratic form $\mathcal{Q}$ on $\mathcal{U}$:

$$\mathcal{Q}(u) =< Lu, u > .$$

Note that in that case the operator L is obtained as the variational derivative of $\mathcal{Q}$:

$$u \mapsto \mathcal{Q}(u) : \quad \delta_u \mathcal{Q}(u) = 2Lu$$

since the first variation is given by

$$\delta \mathcal{Q}(u; v) = 2b(u, v) \text{ for all } u, v \in \mathcal{U}$$

Remark 67 *1.* In case $X = Y = H$ with H a Hilbert space, and H^* is identified with H, then the adjoint $L^* : H \to H$ is uniquely defined from

$$(Lu, v)_H = (u, L^* v)_H \quad \text{for all } u, v \in H.$$

2. Above we defined the adjoint of an operator. When (homogeneous) boundary conditions are present, one can define the adjoint of the operator and the adjoint boundary conditions from

$$\langle Lu, v^* \rangle = \langle u, L^* v \rangle \quad \text{for all} \quad u \in \mathcal{U}^*, \quad v \in \mathcal{V}^*.$$

We will see examples in the following.

In the following we will mainly deal with differential or integral operators.

Exercise 68 *Differential operators*
For a linear differential operator L, the result applied to a (smooth) function u is a function $Lu(x)$ that depends on u and a finite number of derivatives of u at the point x. The order of the highest derivative is called the order of the differential operator.

1. For U functions on the interval $[0, 1]$, and for given functions a, b, c determine the (formal) adjoint of the second order differential operator

$$Lu = a(x)u_{xx} + b(x)u_x + c(x)u.$$

2. Determine conditions on the functions a, b, c that guarantee that L is symmetric.

3. Consider for given function f the following boundary value problem for the operator L above:

$$Lu = f, \quad u(0) = 0, \; u_x(1) = 0.$$

Determine the corresponding adjoint boundary value problem.

4. The generalization to functions of more variables: for U functions on the domain $\Omega \subset R^n$, and for given scalar functions $a, b_1, \dots, b_n, c$, determine the (formal) adjoint of the operator

$$Lu = a(x)\Delta u + \sum_k b_k(x) u_{x_k} + c(x)u.$$

5. Determine the adjoint boundary value problem for this operator with Dirichlet boundary conditions on part of the boundary $\partial\Omega_1$.

Definition 69 *A second order differential operator of the form*

$$Lu = -\partial_x[p(x)\partial_x u] + q(x)u$$

with given scalar functions p, q, is called a Sturm-Liouville operator*.*
The more-dimensional analog is the operator

$$Lu = -div\ [p(x)\ \nabla u] + q(x)u.$$

Proposition 70 *The Sturm-Liouville differential operator is a symmetric operator; it is (half) the variational derivative of the quadratic form*

$$\mathcal{Q}(u) = \int [p(x)u_x^2 + q(x)u^2]dx,$$

and in more dimensions

$$\mathcal{Q}(u) = \int_\Omega [p(x)|\nabla u|^2 + q(x)u^2]dx.$$

Exercise 71 *Integral operators*
For functions on Ω, let $k : \Omega \times \Omega \to R$ be a given function. The integral operator with the function k as kernel is the operator K defined by

$$Ku(x) = \int_\Omega k(x,y)u(y)dy.$$

1. Find the condition for the kernel function k that guarantees that K is a symmetric operator. Detemine in that case the corresponding quadratic form $\mathcal{Q}$, and verify that $\delta\mathcal{Q}(u) = 2K(u)$.

2. Show that the following estimates for $\mathcal{Q}$ can be obtained (when the expressions for k are finite):

- for kernels that are essentially bounded:

  $$|\mathcal{Q}(u)| \leq |k|_\infty \int_\Omega u^2$$

  where $|k|_\infty$ is the sup-norm of k on $\Omega \times \Omega$, and

- for kernels that are square integrable (L_2):

$$|\mathcal{Q}(u)| \leq |K|_{L_2} \int_\Omega u^2 \ \mathit{with} \ \ |K|^2_{L_2} = \int_{\Omega\times\Omega} k^2(x,y)dxdy.$$

3. *Definite kernels.* Show that if the symmetric kernel k is non-negative, then $\mathcal{Q}$ is non-negative: $\mathcal{Q}(u) \geq 0$ for all u.

4. Give a simple example to show that it is not true that when k is positive definite on $\Omega \times \Omega$, the operator K is positive definite. (See the degenerate kernels below.)

5. *Separable kernels.* The kernel k is called separable if it is the product of functions of only one of the variables:

$$k(x,y) = \sum_{m,n=1}^{\infty} a_m(x)b_n(y);$$

when symmetric, this can be written like

$$k(x,y) = \sum_{m,n=1}^{\infty} a_m(x)a_n(y).$$

Describe the range of the integral operator.

6. *Degenerate integral operators*
The symmetric kernel (and the corresponding integral operator) is called degenerate if it is separable with only a finite number of functions:

$$k(x,y) = \sum_{m,n=1}^{N} a_m(x)a_n(y).$$

Show that then K is an operator of finite rank ($\leq N$); in fact determine the range of K.

Integral operators may arise as the inverse of differential operators as is shown in the simplest case in the following example.

Exercise 72 *Integral operator as inverse of differential operator.*
Consider the boundary value problem

$$Lu \equiv -u_{xx} = f, \quad u(0) = u(\pi) = 0,$$

that can be described as the operator equation

$$Lu = f, \quad u \in \mathcal{U}_0 \equiv \{\ u \in C^2 \ \mid \ u(0) = u(\pi) = 0\ \}.$$

1. One can solve this equation in an elementary way; the solution is given by

   $$u = Kf \equiv \int_0^\pi g(x,y)f(y)dy$$

   where K is the symmetric integral operator

   $$\begin{aligned} Kv(x) &= \int g(x,y)v(y)dy, \\ \text{with } g(x,y) &= \begin{cases} (1-y/\pi)x & \text{for} \quad 0 \le x \le y \\ (1-x/\pi)y & \text{for} \quad y \le x \le \pi \end{cases} \end{aligned}$$

   Verify by a direct calculation that this is the unique solution.

2. Derive the solution by direct integration of the differential equation twice and adjusting integration constants to satisfy the homogeneous boundary conditions.

3. Derive the solution also by the method of Greens functions: the right-hand-side as a superposition of pointsources described with Diracs delta-functions, and observe that the kernel $g(x,y)$ is Greens function: the effect at the place x due to a unit force at y.

4. *Relation between the eigenvalues*
   The eigenvalues of L are $\lambda_k = k^2$; the eigenvalues of K are the inverse of those of L, and the eigenfunctions are the same:

   $$L\varphi = \lambda\varphi \Leftrightarrow K\varphi = \mu\varphi \;\; for \;\; \mu = \frac{1}{\lambda}.$$

5. Derive the solution using Fourier-decomposition (which is using the eigenfunction expansion in this case). Conclude that the kernel is non-degenerate and separable, being given by

   $$G(x,y) = \sum_m \frac{\sin mx \, \sin my}{\lambda_m}$$

6. Show that L is bounded from below by λ_1 but, since $\lambda_m \to \infty$ as $m \to \infty$, L is not bounded from above.

7. For K the situation is reversed: K is bounded from above by μ_1; moreover, $\mu_m > 0, \mu_m \to 0$ for $m \to \infty$.

6.1.2 General formulation of EVP

We will now formulate the eigenvalue problem (EVP) in a somewhat more general way, and reformulate it at the same time with two given symmetric quadratic forms instead of with the operators itself.

Let $\mathcal{N}$ be a quadratic form on L_2; we will denote the corresponding operator by N and use the following notation for the corresponding bilinear functional:

$$\mathcal{N}(u) = \langle Nu, u\rangle, \quad \mathcal{N}(u, v) \equiv \langle Nu, v\rangle$$

In the following we want to have $\mathcal{N}$ as a norm, and so we have to assume that $\mathcal{N}$ is positive definite:

$$\mathcal{N}(u) > 0 \quad \textit{for} \;\; u \neq 0.$$

Let $\mathcal{Q}$ be another quadratic form on $\mathcal{U}$, with corresponding symmetric operator L:

$$\mathcal{Q}(u) = \langle Lu, u\rangle, \quad \mathcal{Q}(u, v) \equiv \langle Lu, v\rangle.$$

We will study the eigenvalue problem corresponding to these two operators:

$$Lu = \lambda Nu$$

Note, for $N = Identity$ we recover the standard formulation above; then $\mathcal{N}(u)$ is just the usual L_2-innerproduct. The more general formulation includes the case when we use weighted L_2-norms.

The eigenvalues corresponding to one eigenvalue form a linear space, the *eigenspace* of the eigenvalue, to be denoted by E_λ.
First the result that can be expected for symmetric operators.

Proposition 73 *All eigenvalues are real valued, and the eigen functions can be assumed to be real.*
Eigenfunctions corresponding to different eigenvalues are "orthogonal" with respect to both quadratic forms:

$$\text{for } \varphi \in E_\lambda, \;\; \psi \in E_\mu, \;\; \text{with } \lambda \neq \mu \quad \left\{ \begin{array}{lcl} \mathcal{Q}(\varphi, \psi) & = & 0 \\ \mathcal{N}(\varphi, \psi) & = & 0. \end{array} \right.$$

We can denote this for the eigenspaces as[2]

$$E_\lambda \perp_{\mathcal{N}} E_\mu, \quad E_\lambda \perp_{\mathcal{Q}} E_\mu \text{ when } \lambda \neq \mu.$$

---

[2] Be carefull with this (useful) description: since $\mathcal{N}$ is a norm, orthogonality can be understand in the ususal sense; however $\mathcal{Q}$ is not necessarily positive; when it is not positive the use of the word "orthogonal" may be somewhat misleading.

The eigenvalue problem for $\mathcal{Q}$ and $\mathcal{N}$ can then equivalently be defined as the problem to find eigenfunctions $\varphi \in H, \varphi \neq 0$, such that for some eigenvalue λ:

$$\mathcal{Q}(\varphi, v) = \lambda \mathcal{N}(\varphi, v) \quad \textit{for all } v \in \mathcal{U}.$$

Since this can be rewritten like

$$\delta\mathcal{Q}(u; v) = \lambda\delta\mathcal{N}(u; v),$$

one interpretation of an eigenfunction with eigenvalue λ is as a critical point of the functional

$$\mathcal{U} \ni u \to \mathcal{Q}(u) - \lambda\mathcal{N}(u).$$

However, since λ is not given, but has to be found, this is not a very useful attack. Much more fruitful is to interpret λ as a multiplier appearing from a constrained problem.

Proposition 74 *(Normalized) Eigenfunctions φ are critical points of:*

$$\varphi \in \{\mathcal{Q}(u) \mid u \in U, \ \mathcal{N}(u) = 1\}.$$

Equivalently,

$$\varphi \in \{\mathcal{R}(u) \mid u \in U\}, \textit{with } \mathcal{R}(u) = \frac{\mathcal{Q}(u)}{\mathcal{N}(u)}.$$

where $\mathcal{R}$ is the so-called Rayleigh quotient. *The corresponding eigenvalues are precisely the critical values $\mathcal{R}(\varphi)$.*

This formulation will be most useful, as we will see. It will determine the principal eigenvalue (the largest or smallest one) if $\mathcal{R}$ attains its maximum or minimum. Other eigenfunctions can then be found in a recursive, or non-recursive way, all based on the constrained variational formulation above.

When exploiting the variational characterization of the eigenfunctions with the Rayleigh quotient, one has to distinguish between differential and integral operators. If $\mathcal{Q}$ corresponds to a differential operator L, in most cases $\mathcal{Q}$ is *strongly coercive* (or elliptic) with respect to $\mathcal{N}$, meaning that the Rayleigh-quotient is bounded from below but not from above: for some $\gamma \in \mathcal{R}$

$$\mathcal{R}(u) \geq \gamma, \ \textit{and for some sequence } u_m, \ \mathcal{R}(u_m) \to \infty.$$

Exercise 75

1. If $\gamma > 0$, Q defines a norm itself, and the assumption of ellipticity means that this norm is stronger (not equivalent) than the N-norm.

2. Show that on $U_0 = \{u(0) = u(\pi) = 0\}$ the norm $Q(u) = \int u_x^2$ is coercive with respect to $N(u) = \int u^2$.

3. If R is not definite (then $\gamma < 0$) the quadratic form Q is not a norm; by defining

$$\bar{\mathcal{Q}}(u) := \mathcal{Q}(u) + 2|\gamma|\mathcal{N}(u)$$

it follows that $\bar{\mathcal{Q}}(u) \geq |\gamma| N(u)$, and so is a norm that is stronger than N. Since the eigenfunctions of Q and $\bar{\mathcal{Q}}$ are the same, and the eigenvalues just differ the constant shift 2γ, one could just as well study the eigenvalue problem for $\bar{\mathcal{Q}}$ and N. Stated differently, it would be no restriction to assume Q to be positive definite from the start on.

4. Show that the Sturm-Liouville operator with

$$\mathcal{Q}(u) = \int p(x) u_x^2 + q(x) u^2$$

is coercive on U_0 with respect to $N = \int \rho u^2$ provided p is non-negative (and non-trivial), q is bounded, and ρ is positive definite.

The unboudedness of differential operators is different from integral operators (that have a kernel that is essentially bounded or square integrable) since then the Raylegh quotient is bounded: for some $\sigma > 0$

$$|\mathcal{R}(u)| \leq \sigma.$$

This will explain the reason why for differential operators we minimize the Rayleigh quotient, and for integral operators maximize it (or its absolute value).

6.2 Spectral theorem for differential operators

Theorem 76 Principal eigenfunction and -value
Suppose that $\mathcal{Q}$ is coercive (elliptic) with respect to $\mathcal{N}$: for some $\gamma (> 0)$

$$\mathcal{Q}(u) \geq \gamma \mathcal{N}(u),$$

and assume that the minimization problem for $\mathcal{R}$ has a solution. Then the solution

$$\varphi_1 \in Min \ \{\mathcal{Q}(u) \ \ |u \in \mathcal{U}, \ \mathcal{N}(u) = 1\} \sim Min \{\mathcal{R}(u) \ |u \in \mathcal{U}\}$$

is the principal eigenfunction φ_1, *i.e. the eigenfunction corresponding to the smallest eigenvalue, the* principal eigenvalue, λ_1 *that is given by*

$$\lambda_1 = \mathcal{R}(\varphi_1) \ (\geq \gamma).$$

Any other eigenfunction (independent of φ_1) can be assumed to be orthogonal (both in $\mathcal{N}$-, as well as in $\mathcal{Q}$-sense) to φ_1. In the following formulation this will be exploited in a successive way.

Theorem 77 Successive characterization
The eigenfunctions and eigenvalues can be obtained in a successive way: if $\varphi_1, \ldots, \varphi_k$ *are the eigenfunctions corresponding to the eigenvalues that are ordered like*

$$(\gamma \leq)\ \lambda_1 \leq \lambda_2 \ldots \leq \lambda_k,$$

the "next" eigenfunction is found as the solution of

$$\varphi_{k+1} \in Min\ \left\{\mathcal{Q}(u)\ \middle| u \in H, \mathcal{N}(u) = 1, \mathcal{N}(u, \varphi_j) = 0,\ for\ 1 \leq j \leq k\right\};$$

the corresponding eigenvalue $\lambda_{k+1} \equiv \mathcal{R}(\varphi_{k+1})$ *"follows"* λ_k *in the sense that* $\lambda_{k+1} \geq \lambda_k$*, while, when* $\lambda_{k+1} > \lambda_k$*, there are no other eigenvalues inbetween.*

Exercise 78

1. The orthogonality constraints in the successive characterization are natural constraints: although essential in the definition of the constraint set, there is no effect in the equation for the critical point: the corresponding multiplier vanishes.
   To verify this, consider the equation for

   $$\psi \in Crit\ \{\mathcal{R}(u)\ | u \in H, \mathcal{N}(u, f) = 0\}$$

   where f is any given function. The governing equation is for some multipliers μ, σ

   $$L\psi = \mu N\psi + \sigma f, \quad \text{with} \quad \mu = \mathcal{R}(\psi).$$

   Verify that $\sigma = 0$ if f is some eigenfunction, but not so in general.

2. By its nature, the above formulation requires the knowledge of the previous eigenfunctions to find the next eigenvalue: the eigenvalue λ_{k+1} follows by investigating the minimizer of $\mathcal{R}$ on the set of functions orthogonal to the previous eigenfunctions. When one wants to use this formulation in a numerical procedure, for instance, this may lead to serious error-accumulation: in calculating λ_1, an error in the calculation of φ_1 influences the constraint set for λ_2 and induces an additional error in the calculation of λ_2 and of φ_2, and so on. This can be seen more quantitatively as follows.

3. Suppose that in a numerical calculation an approximation $\hat{\varphi}_1$ for the first eigenfunction φ_1 is constructed that is correct up to order ε (in $\mathcal{N}$-norm for instance):

   $$\varphi_1 - \hat{\varphi}_1 = \mathcal{O}(\varepsilon).$$

   Show that then the approximate first eigenvalue $\hat{\lambda}_1$ that is constructed is correct up to order ε^2:

   $$\lambda_1 - \hat{\lambda}_1 = \mathcal{O}(\varepsilon^2).$$

4. Investigate the effect of an error ε in the calculation of φ_1 for the approximation of λ_2 and of φ_2. Do the same for higher eigenvalues and eigenfunctions.

The conclusion must be that the successive characterization as given above is not very suitable for numerical calculation of the successive eigenvalues and eigenfunctions. In a next section we will consider a non-successive characterization that is free of error-accumulation.

Just as for symmetric matrices, the eigenfunctions form a complete set; this is a very strong result in infinite dimensions but requires some additional compactness condition. The proof will be based on the successive characterization, but actually only requires the knowledge that the eigenvalues can be ordered and tend to infinity (are not bounded above). This is usually the case for differential operators when $\mathcal{Q}$ defines a norm that is "essentially stronger" than $\mathcal{N}$[3].

Theorem 79 Completeness of the set of eigenfunctions

If each eigenvalue has finite multiplicity, and if the eigenvalues are unbounded:

$$(\gamma \leq)\ \lambda_1 \leq \lambda_2 \ldots \leq \lambda_k \ldots \to \infty,$$

then the set of eigenfunctions is complete, both with respect to the $\mathcal{N}$-norm and with respect to the $\mathcal{Q}$-norm[4].

Generalized Fourier theory

The completeness result implies that any function in $\mathcal{U}$ can be written as a (generalized) *Fourier series*

$$u(x) = \sum_1^\infty u_m \varphi_m(x);$$

using the fact that the eigenfunctions are orthonormal, it follows directly that the *Fourier coefficients* are given by

$$u_m = \mathcal{N}(u, \varphi_m);$$

the infinite sum converges in the sense that

$$\mathcal{N}(u - \sum_1^M u_m \varphi_m) \to 0 \quad \textit{for} \;\; M \to \infty$$

and also in the stronger norm

$$\mathcal{Q}(u - \sum_1^M u_m \varphi_m) \to 0 \quad \textit{for} \;\; M \to \infty.$$

---

[3] With the functional analytic notions of Chapter ??, it should hold that $\mathcal{N}$ is weakly continuous with respect to $\mathcal{Q}$: any sequence bounded in $\mathcal{Q}$-norm should have a subsequence that converges in $\mathcal{N}$-norm; in these cases it can be *proved* that all eigenvalues have finite multiplicity and that the eigenvalues are unbounded from above.

[4] When $\mathcal{Q}$ is not definite, this should be understood with respect to the $\bar{\mathcal{Q}}$-norm, with $\bar{\mathcal{Q}} = \mathcal{Q} + (|\lambda_1| + \varepsilon)\mathcal{N}$, for any $\varepsilon > 0$.

Fredholm alternative

Another interpretation is that the operator L is in *diagonal form* with respect to a basis of eigenfunctions, and hence that the inverse of L can be found easily. For simplicity suppose that $N = Identity$, and consider the inhomogeneous problem

$$Lu = f, \quad u \in \mathcal{U}.$$

Writing $f = \sum f_n \varphi_n$, with f_n the Fourier coefficients of f, the solution is given by

$$u = \sum_m \frac{f_m}{\lambda_m} \varphi_m,$$

at least when

- *either* all eigenvalues λ_m are non-zero (the operator L is invertible),
- *or*, if there is a zero eigenvalue, with eigenspace

  $$E_{\lambda=0} \text{ (consisting of the eigenfunctions with eigenvalue } 0\text{)},$$

  there exists a solution only if the inhomogeneous term satisfies the orthogonality conditions

  $$f \perp E_{\lambda=0};$$

  in that case the solution is not unique: any element from $E_{\lambda=0}$ can be added.

These results are just a straightforward generalization of the *Fredholm alternative* for (symmetric) matrices.

Inverse as integral operator with Greens function as kernel

Assuming all eigenvalues to be non-zero, the solution $u = \sum_m \frac{f_m}{\lambda_m} \varphi_m$, can be written by expanding the Fourier coefficients of f explicitly, and the result is

$$Lu(x) = f(x) \Leftrightarrow u(x) = \int G(x, y) f(y) dy,$$

where $G(x, y) = G(y, x)$ is the so-called *Greens function*, given by

$$G(x, y) \sum_m \frac{1}{\lambda_m} \varphi_m(x) \varphi_m(y).$$

Hence, the inverse of L is an integral operator with G as (symmetric) kernel.

6.2.1 Examples

The first example shows that the results for the EVP for specific operators are generalizations of the ususal Fourier theory.

EVP for Sturm-Liouville problems on an interval
For given positive functions ρ and p, and a function q on $[0,\pi]$ (all smooth), the Sturm-Liouville eigenvalue problem (with Dirichlet boundary conditions) reads:

$$L\varphi = -\partial_x(p(x)\varphi_x) + q(x)\varphi = \lambda\rho(x)\varphi, \quad \varphi(0) = \varphi(1) = 0,$$

and is obtained in $\mathcal{U}_0 = \{u \in L_2 \mid u(0) = u(\pi) = 0\}$ with the quadratic forms

$$\mathcal{N}(u) = \int \rho(x)u^2, \quad \mathcal{Q}(u) = \int [p(x)u_x^2 + q(x)u^2].$$

Exercise 80 *1.* The special case $\rho \equiv 1, p \equiv 1, q \equiv 0$ provides Fourier theory (for functions that are odd on $[-\pi,\pi]$):
then the eigenvalues and (normalized) corresponding eigenfunctions are given by

$$\lambda_m = m^2, \quad \varphi_m = \sqrt{2/\pi}\sin mx, \quad m \geq 1.$$

The completeness result in the spectral theorem implies that any function satisfying the boundary conditions can be written as a Fourier-sine series

$$u(x) = \sqrt{2/\pi}\sum_1^\infty u_m \sin mx,$$

for Fourier coefficients given by

$$u_m = \langle u, \varphi_m\rangle = \sqrt{2/\pi}\int u(x)\sin mx dx;$$

the convergence in the N-norm is just the usual L_2-norm:

$$\int (u - \sum_1^M u_m\varphi_m(x))^2 dx \to 0, \quad \text{for } M \to \infty.$$

The convergence in the Q-norm implies a much stronger statement. To investigate that, exploit the *Poincaré inequality:* for some constant $c_1 > 0$ it holds that

$$|u|_\infty^2 \leq c_1 \int u_x^2 \quad \text{for all} \quad u, \; u(0 = u(\pi) = 0.$$

Then the convergence in the Q-norm implies the *pointwise* convergence of the Fourier-sine series:

$$|u - \sum_1^M u_m\varphi_m(x)|_\infty \to 0, \; \text{for} M \to \infty.$$

2. Changing the boundary conditions to Neumann boundary conditions:

$$u_x(0) = u_x(\pi) = 0$$

provides *Fourier cosine series,* since then

$$\lambda_m = m^2, \quad \varphi_m = \sqrt{2/\pi}\cos mx, \quad m \geq 0;$$

completeness in L_2-norm, and pointwise, in the same way as above.

3. Observe that in both cases the eigenvalues are "simple": to each eigenvalue there corresponds precisely one eigenfunction; equivalently: the eigenspaces are one-dimensional. This is characteristic for Sturm-Liouville eigenvalue problems on an *interval,* as we will prove later.

EVP for Sturm-Liouville problems on a spatial domain

For a domain $\Omega \subset \mathcal{R}^n$, with boundary $\partial\Omega = \partial\Omega_D \cup \partial\Omega_N$, and for given functions $p(x), q(x)$ and $\rho(x)$, the quadratic forms

$$\mathcal{N}(u) = \int_\Omega \rho u^2, \quad \mathcal{Q}(u) = \int_\Omega p(x)|\nabla u|^2 + q(x)u^2$$

on the set

$$\mathcal{U} = \{\ u : \Omega \in \mathcal{R}\ \mid\ u(x) = 0 \ \ for\ \ x \in \partial\Omega_D\ \}$$

leads to the EVP

$$\begin{aligned} -\mathrm{div}\ (p(x)\nabla\phi) + q(x)\phi &= \lambda\phi \ \text{ in } \ \Omega \\ \phi &= 0 \ \text{ on } \partial\Omega_D \\ p(x)\partial_n\phi &= 0 \ \text{ on } \partial\Omega_N \end{aligned}$$

Sufficient conditions on the functions p, ρ that make it possible to apply the general theory are that they are positive definite:

$$p(x) \geq p_0 > 0, \quad \rho(x) \geq \rho_0 > 0.$$

Then existence and completeness follows.
(It should be noted that in more dimensions ($n \geq 2$) the convergence in $\mathcal{Q}$-norm does *not* imply pointwise convergence; only for functions of one variable the Poincaré inequality holds!)

Exercise 81 In a few specific cases, for special domains Ω, the eigenfunctions can be found explicitly. In all these cases the *method of separation of variables* is used.
In the following we consider the EVP for the Laplace operator: $p \equiv 1, q \equiv 0, \rho \equiv 1$, so

$$\mathcal{N}(u) = \int_\Omega u^2, \quad \mathcal{Q}(u) = \int_\Omega |\nabla u|^2$$

and

$$\begin{aligned} -\Delta\phi &= \lambda\phi \quad \mathit{in}\ \ \Omega \\ \phi &= 0 \quad \mathit{on}\ \partial\Omega_D \\ \partial_n\phi &= 0 \quad \mathit{on}\ \partial\Omega_N \end{aligned}$$

1. ***EVP for Laplacian on a square***
   If $\Omega = [0,a]\times[0,b]$ is a square in the plane, and either Dirichlet or Neumann boundary values hold on each side, eigenfunctions are found by separation of variables $u(x,y) = U(x)V(y)$. For instance, for Dirichlet condition on the whole boundary, one finds eigenvalues and eigenfunctions

   $$\begin{aligned} \lambda_{k,m} &= \left(\frac{k\pi}{a}\right)^2 + \left(\frac{m\pi}{b}\right)^2 \\ \phi_{k,m} &= \sin\left(\frac{k\pi}{a}\right)x\sin\left(\frac{m\pi}{b}\right)y, \quad k,m \geq 1 \end{aligned}$$

   Note that the principal eigenfunction is sign-definite on Ω. Furthermore, if the lengths a and b are rationally dependent, $\frac{a}{b} \in Rt$, there are eigenvalues that are non-simple; for instance, if $a = b, \lambda_{k,m} = \lambda_{m,k}$ for all k, m. On the other hand, when they are rationally independent, all eigenvalues are simple.

2. ***EVP for Laplacian on a disc: Fourier-Bessel theory***
   Consider the unit disc $\Omega = D \equiv \{x \mid |x| \leq 1\}$ with Dirichlet boundary condition:

   $$\mathcal{U}_0 = \{\ u : D \to \mathcal{R}\ \mid\ u(x) = 0 \ \text{ for } \ |x| = 1\ \}$$

   It is natural to introduce polar coordinates $(r,\phi) \in R_+ \times S^1$ and consider $u = u(r,\phi)$. The quadratic forms are then given by

   $$\begin{aligned} \mathcal{N}(u) &= \textstyle\int u^2 r dr d\phi \\ \mathcal{Q}(u) &= \textstyle\int [u_r^2 + \frac{1}{r^2}u_\phi^2] r dr d\phi \end{aligned}$$

   and the eigenvalue problem reads

   $$\begin{aligned} -\Delta u &\equiv -\left[\frac{1}{r}\partial_r\left(r\partial_r u\right) + \frac{1}{r^2}\partial_\phi^2 u\right] = \lambda u, \quad \mathit{for}\ r < 1 \\ u &= 0 \quad \mathit{for}\ r = 1 \end{aligned}$$

   Separation of variables: writing $u(r,\phi) = V(r)\Phi(\phi)$ leads to

   $$-\frac{1}{r}\partial_r(rV_r)\Phi - \frac{1}{r^2}V(r)\partial_\phi^2\Phi = \lambda V\Phi,$$

and hence for some constant α

$$-\partial_\phi^2 \Phi = \alpha\Phi, \text{ and } -\frac{1}{r}\partial_r(rV_r) + \frac{\alpha}{r^2}V(r) = \lambda V.$$

Periodicity in $\phi \in [0, 2\pi]$ requires that $\alpha = k^2, k = 0, 1, \ldots,$ for which

$$\Phi = \Phi_m = a\cos m\phi + b\sin m\phi, \quad m = 0, 1, \ldots .$$

Remains to investigate the equation for V, which is a EVP in the radial variable only:

$$-\frac{1}{r}\partial_r(rV_r) + \frac{m^2}{r^2}V(r) = \lambda V.$$

Solutions of this equation can be written with Bessel functions (see Exercise 6.)
The solution that is bounded at $r = 0$ is given by

$$V(r) = J_k(\sqrt{\lambda}r).$$

To satisfy the boundary condition $V(r = 1) = 0$, it follows that λ should satisfy for certain $\ell \geq 1$

$$\lambda = \lambda_{k,\ell} = \sigma_{k,\ell}^2,$$

where $\sigma_{k,\ell}$ is the $\ell-$the zero of the Bessel function J_k. Then we find as eigenfunctions

$$\psi_{m,\ell} = J_m(\sigma_{m,\ell}r)\ [a\sin m\phi + b\cos m\phi], m \geq 0, \ell \geq 1.$$

Special case: Radially symmetric solutions
Consider the eigenfunctions that are independent of the angle variable ϕ:

$$\lambda_{0,\ell} = \sigma_{0,\ell}^2, \quad \psi_{0,\ell} = J_0(\sigma_{0,\ell}), \ell \geq 1.$$

These are the eigenfunctions of the EVP

$$-\frac{1}{r}\partial_r(rv_r) = \lambda v,$$

corresponding to the quadratic forms

$$\mathcal{N}_0(v) = 2\pi\int v^2 r dr, \quad \mathcal{Q}_0(v) = 2\pi\int(\partial_r v)^2 r dr.$$

Orthogonality with respect to the $\mathcal{N}$-innerproduct implies that

$$\int_0^1 J_0(\sigma_{0,k}r)J_0(\sigma_{0,m}r)rdr = 0, \quad \text{for } k \neq m.$$

Completeness implies that any function $v(r)$, with $v(0)$ finite and $v(1) = 0$, can be written like a so-called *Fourier-Bessel series*

$$v(r) = \sum_{\ell \geq 1} v_\ell J_0(\sigma_{0,\ell} r),$$

where the Fourier-Bessel coefficients are given by

$$v_\ell = \frac{\int v(r) J_0(\sigma_{0,\ell} r) r dr}{\int J_0(\sigma_{0,\ell} r)^2 r dr}.$$

The convergence is with respect to the $\mathcal{N}_0$ and the $\mathcal{Q}_0$-norm.

6.2.2 Proof of the spectral theorem

Proof of Theorem 76
We only have to prove that there is no eigenvalue μ smaller than λ_1. If $\psi \in \mathcal{U}$ is the eigenfunction with eigenvalue μ, then $\mathcal{R}(\psi) = \mu$; the minimizing property of λ_1 then implies the required result: $\mu \geq \lambda_1$. □

Proof of Theorem 77
From Ex. Refexerracc it follows already that the constained minimizers are all eigenfunctions. So, it only remains to show that if $\lambda_{k+1} > \lambda_k$, then there is no eigenvalue μ inbetween. Suppose $\lambda_k < \mu$, and ψ is an eigenfunction corresponding to μ. Then ψ is perpendicular to the eigenfunctions $\varphi_1, \dots, \varphi_k$. Hence, ψ belongs to the constrained set in the characterization of λ_{k+1}, and hence by the minimality property of λ_{k+1}, it follows that necessarily $\mu \equiv \mathcal{R}(\psi) \geq \lambda_{k+1}$, and hence the result. □.

Proof of Theorem 79
Completeness in $\mathcal{N}$-norm
For fixed N, any function u can be written as its projection (in $\mathcal{N}$- innerproduct) on the linear span of the first N eigenfunctions (assumed to be normalized in the $\mathcal{N}$-norm for simplicity) and a remainder like

$$u = \sum_1^N \alpha_k \varphi_k + \rho_N$$

where α_k are the Fourier coefficients, determined by

$$\text{Min} \left\{ \mathcal{N}(u - \sum_1^N \alpha_k \varphi_k) \mid \alpha_1, \dots, \alpha_N \right\},$$

explicitly given by $\alpha_k = \mathcal{N}(u, \varphi_k)$. The remainder is orthogonal to the linear span:

$$\mathcal{N}(\varphi_k, \rho_N) = 0, 1 \leq k \leq N.$$

Then

$$\mathcal{N}(\rho_N) = \mathcal{N}(u) - \sum_1^N \alpha_k^2,$$

and completeness in the $\mathcal{N}$-norm means that

$$\mathcal{N}(\rho_N) \to 0 \quad \textit{for} \;\; N \to \infty.$$

In order to show this, observe that from the extremal property of λ_N (assumed to be positive, which is the case for N sufficiently large), and $\mathcal{N}(\varphi_k, \rho_N) = 0, 1 \leq k \leq N$, it follows that $\mathcal{R}(\rho_N) \geq \lambda_N$, and thus

$$\mathcal{N}(\rho_N) \leq \frac{1}{\lambda_N} \mathcal{Q}(\rho_N).$$

Since $\lambda_N \to \infty$ for $N \to \infty$, the result is obtained if we show that $\mathcal{Q}(\rho_N)$ is uniformly bounded: $\mathcal{Q}(\rho_N) \leq A$ for $N \to \infty$.
To prove the uniform boundedeness, use $\mathcal{Q}(\varphi_k) = \lambda_k$, $\mathcal{Q}(\rho_N, \varphi_N) = 0$, and hence

$$\mathcal{Q}(u) = \sum_1^N \alpha_k^2 \lambda_k + \mathcal{Q}(\rho_N),$$

from which it follows that

$$\mathcal{Q}(\rho_N) = \mathcal{Q}(u) - \sum_1^N \alpha_k^2 \lambda_k \leq \mathcal{Q}(u) - \lambda_1 \sum_1^N \alpha_k^2$$

$$\leq \mathcal{Q}(u) + |\lambda_1| \mathcal{N}(u) =: A,$$

and hence the result. □

Completeness in $\mathcal{Q}$-norm
Without restriction we can assume that $\mathcal{Q}$ is positive definite (if necessary, add $2|\lambda_1|\mathcal{N}$). Completeness with respect to $\mathcal{Q}$ means that

$$\mathcal{Q}(\rho_N) \to 0 \quad \textit{for}\; N \to \infty.$$

To show that this is the case, first observe that

$$0 \leq \mathcal{Q}(\rho_N) = \mathcal{Q}(u) - \mathcal{Q}(u_N), \;\; \textit{where} \;\; u_N \equiv \sum_1^N \alpha_k \varphi_k.$$

Since $N \to \mathcal{Q}(u_N)$ is a sequence, non-decreasing and bounded above (by $\mathcal{Q}(u)$), there exists a limit:

$$\mathcal{Q}(u_N) \to \mathcal{Q}(v) \leq \mathcal{Q}(u),$$

where

$$v = \sum_{1}^{\infty} \alpha_k \varphi_k$$

is the limit in the $\mathcal{N}$-norm. From the completeness in $\mathcal{N}$-norm, it follows that $\mathcal{N}(u) = \mathcal{N}(v)$. Since also in the limit $\mathcal{Q}(u - v) = \mathcal{Q}(u) - \mathcal{Q}(v) \geq 0$, it would follow that necessarily $u = v$, and hence completeness in $\mathcal{Q}$-norm, provided it can be shown that

$$\mathcal{Q}(u) = \mathcal{Q}(v), \ \textit{or} \ \mathcal{R}(u) = \mathcal{R}(v).$$

To show this, reason by contradiction. Assuming $\mathcal{R}(v) < \mathcal{R}(u)$, it follows that $u = v + \xi$ with $\mathcal{R}(\xi) = \mathcal{R}(u) - \mathcal{R}(v) > 0$. Then $\xi \neq 0$, and satisfies

$$\mathcal{Q}(\xi, \varphi_k) = \mathcal{N}(\xi, \varphi_k) = 0 \quad \textit{for all } k \in N.$$

From the successive characterization of the eigenvalues it then follows that $\mathcal{R}(\xi) \geq \lambda_n$ for all n. This contradicts the fact that $\lambda_n \to \infty$ for $n \to \infty$, while $\mathcal{R}(\xi)$ is finite, and hence the completeness result. □

6.3 Comparison methods for principal eigenvalues

Often we want to compare the eigenvalues of two different eigenvalue problems. When for each problem the eigenvalues are found in a variational way, this may be done in an elegant way. The eigenvalue problems to be compared may differ in three ways (or combinations thereof)

- the operators are different,
- the boundary conditions are different,
- the domain of definition of the functions is different.

Exercise 82 Consider the vibrations of a linear string governed by

$$u_{tt} = \partial_x(\sigma(x) u_x), \quad u(0, t) = u(\ell, t) = 0,$$

where ℓ is the length, and σ is a material property. When looking for time-harmonic solutions of the form

$$u(x, t) = v(x) \exp[i\omega t]$$

there results the eigenvalue problem for v with $\omega^2 = \lambda$:

$$-\partial_x(\sigma(x) v_x) = \lambda v, \quad v(0) = v(\ell) = 0.$$

The principal eigenvalue λ_1 determines the lowest frequency of vibration of the string; in practise it determines the fundamental tone of a piano etc. Of course, its value depends on the length ℓ, on the material properties described by σ, and in fact also on the boundary conditions.

1. For σ is constant, the principal eigenvalue is given by

   $$\lambda_1 = \sigma(\frac{\pi}{\ell})^2 \text{ with eigenfunction } \varphi_1 = \sin(\frac{\pi x}{\ell}).$$

   Hence, the principal eigenvalue decreases when the length increases, and/or when the tension σ decreases.

2. For a string with a free endpoint at $x = \ell$, the boundary conditions are replaced by $v(0) = 0, v_x(\ell) = 0$. Then the principal eigenvalue μ_1 is given by

   $$\mu_1 = \sigma(\frac{\pi}{2\ell})^2, \quad \text{with eigenfunction } \psi_1 = \sin(\frac{\pi x}{2\ell})$$

   and produces a lower fundamental tone since $\mu_1 < \lambda_1$.

3. The same result holds true for the non-fundamental eigenvalues:

   $$\lambda_m = \sigma(\frac{m\pi}{\ell})^2, \quad \text{with eigenfunction } \varphi_m = \sin(\frac{m\pi x}{\ell}),$$

   $$\mu_m = \sigma(\frac{m\pi}{2\ell})^2, \quad \text{with eigenfunction } \psi_m = \sin(\frac{m\pi x}{2\ell});$$

   note that $\mu_m < \lambda_m$ for all $m \geq 1$.

4. The physical statement of these results is that *upon relaxing the constraints, the eigenvalues decrease.*

Using the extremal characterization for the principal eigenvalue, comparison between different problems may be relatively easy. For ease of presentation we will mainly deal with differential operators for which the principal eigenvalue *minimizes* the Rayleigh quotient.

Proposition 83 *Let $\mathcal{U}$ be the linear space, and $\mathcal{R}$ the Rayleigh quotient. Suppose that the principal eigenvalue Λ minimizes $\mathcal{R}$ on $\mathcal{U}$; making its dependence explicitly, we write*

$$\Lambda(\mathcal{R},\mathcal{U}) = Min\{\mathcal{R}(u) \mid u \in \mathcal{U}\}$$

Then Λ depends monotononically on $\mathcal{R}$ and on $\mathcal{U}$ in the following senses:

- $\Lambda(\mathcal{R}_1,\mathcal{U}) \leq \Lambda(\mathcal{R}_2,\mathcal{U})$ if $\mathcal{R}_1(u) \leq \mathcal{R}_2(u)$ for all $u \in \mathcal{U}$
- $\Lambda(\mathcal{R},\mathcal{U}_1) \leq \Lambda(\mathcal{R},\mathcal{U}_2)$ if $\mathcal{U}_1 \supset \mathcal{U}_2$.

Proof. The first statement follows from

$$\mathcal{R}_1(u) \leq \mathcal{R}_2(u) \quad \textit{for all} \;\; u \in \mathcal{U}$$

$$\Longrightarrow \text{ Min } \{\mathcal{R}_1(u) | u \in \mathcal{U}\} \leq \mathcal{R}_2(u) \quad \textit{for all} \;\; u \in \mathcal{U}$$

$$\Longrightarrow \text{ Min } \{\mathcal{R}_1(u) | u \in \mathcal{U}\} \leq \text{Min } \; \{\mathcal{R}_2(u) | u \in \mathcal{U}\}.$$

The second statement from the fact that the minimizer decreases (or at least does not increase) if the domain of definition is enlarged ("relaxing the constraints ..."). □.

Exercise 84 Sturm-Liouville comparison results

1. *Different operators*
   Let $\Lambda_{1,2}$ be the principal eigenvalue of respectively

   $$-\text{div } [p_1(x)\nabla u] + q_1(x)u = \Lambda_1 \rho_1 u,$$

   $$-\text{div } [p_2(x)\nabla u] + q_2(x)u = \Lambda_2 \rho_2 u$$

   on a domain Ω with the same boundary conditions. If

   $$p_1 \leq p_2, \quad q_1 \leq q_2, \quad \rho_1 \geq \rho_2 \quad \textit{on} \;\; \Omega,$$

   the Rayleigh quotients satisfy

   $$\mathcal{R}_1(u) \equiv \frac{\int [p_1 |\nabla u|^2 + q_1 u^2]}{\int \rho_1 u^2} \leq \frac{\int [p_2 |\nabla u|^2 + q_2 u^2]}{\int \rho_2 u^2} \equiv \mathcal{R}_2(u),$$

   and hence $\Lambda_1 \leq \Lambda_2$.

2. *Different boundary conditions*
   For the same S-L operator on Ω, consider two different boundary conditions

   $$\begin{aligned} u &= 0 \text{ on } \partial\Omega_1, \;\; \& \;\; \partial_n u = 0 \text{ on } \partial\Omega/\partial\Omega_1 \\ u &= 0 \text{ on } \partial\Omega_2, \;\; \& \;\; \partial_n u = 0 \text{ on } \partial\Omega/\partial\Omega_2 \end{aligned}$$

   It should be noted now that the Neumann boundary conditions arise as natural boundary conditions; hence the correct boundary conditions are obtained by investigating the Rayleigh quotient on the sets

   $$\mathcal{U}_{1,2} = \{ \; u \;\; | \;\; u = 0 \;\; \textit{on} \;\, \partial\Omega_{1,2} \; \}.$$

   When $\partial\Omega_1 \subset \partial\Omega_2$ ("relaxing ..."), it holds that $\mathcal{U}_1 \supset \mathcal{U}_2$, and hence $\Lambda_1 \leq \Lambda_2$.

3. *Different domains, Dirichlet boundary conditions*
   Consider the same S-L operator with Dirichlet boundary condition on two domains $\Omega_2 \subset \Omega_1$ (the functions are defined on the largest domain, and so is the Rayleigh quotient). Any function $v_2 \in \mathcal{U}_2 = \{ \, v : \Omega_2 \ \mid \ v = 0 \ on \partial\Omega_2 \, \}$ can be extended to a function v_1 on Ω_1 by assigning it the value zero for $x \in \Omega_1/\Omega_2$; this defines the space of functions $\bar{\mathcal{U}_1} = \{ \, v : \Omega_1 \ \mid \ v = 0 \ forx \in \Omega_1/\Omega_2 \, \}$. Since extension with zero does not change the value of the Rayleigh quotient, $\mathcal{R}(v_1) = \mathcal{R}(v_2)$, and since $\bar{\mathcal{U}_1} \subset \mathcal{U}_1 = \{ \, u : \Omega_1 \ \mid \ u = 0 \ on\partial\Omega_1 \, \}$, it follows that

$$\begin{aligned} \Lambda_2 &= \text{Min } \{\mathcal{R}(v_2) | \ v_2 \in \mathcal{U}_2\} = \text{Min } \{\mathcal{R}(v_1) | \ v_1 \in \mathcal{U}_1\} \\ &\geq \text{Min } \{\mathcal{R}(u) | \ u \in \mathcal{U}_1\} = \Lambda_1 \end{aligned}$$

Remark 85 It should be noted that the inequalities derived above for the principal eigenvalue cannot so easily be extended to non-principal eigenvalues. The reason is that, for instance for the second eigenvalue, $\mathcal{R}$ has to be invesigated on the functions orthogonal to the first eigenfunction. When dealing with two problems, the principal eigenfunctions, say Φ_1 and Ψ_1, will differ, and so will their orthogonal complements:

$$\{ \, u \ \mid u \in \mathcal{U}, \ \mathcal{N}(u, \Phi_1) = 0 \, \} \neq \{ \, u \ \mid u \in \mathcal{U}, \ \mathcal{N}(u, \Psi_1) = 0 \, \}$$

while one is not simply included in the other. Hence, no conclusions can be drawn by considering the mimization problems, not even for the same $\mathcal{R}$:

$$Min \ \{\mathcal{R}(u) | \mathcal{N}(u, \Phi_1) = 0\} = \ ?? \ = Min \ \{\mathcal{R}(u) | \mathcal{N}(u, \Psi_1) = 0\}$$

and hence no conclusions for the second eigenvalue.
This situation motivates the characterization of the second (and higher) eigenvalue without using the first eigenfunction; in the next section we will describe such a non-successive characterization.

6.4 Non-successive characterizations of eigenvalues

Recall the two reasons we have encountered until now to look for non-successive characterizations for eigenvalues: the error-accumulation when using numerical approximations, and the comparison of non-principal eigenvalues described above.

6.4.1 Min-max and Max-Min formulations

Formulation and notation
Starting point are the quadratic forms $\mathcal{N}$ and $\mathcal{Q}$, and the eigenvalues λ_k and

eigenfunctions φ_k that are found from the successive characterization; for definiteness we assume that they are defined in a successive minimizing way, as for differntial operators.

Both functionals $\mathcal{Q}$ and $\mathcal{N}$ are defined on the linear space $\mathcal{U}$; for many applications it is important to be able to deal with another space, denoted by $\mathcal{W}$, that is such that $\mathcal{U} \subset \mathcal{W}$ and such that $\mathcal{N}$ is also defined on $\mathcal{W}$.

For $n \in I\!N$ we consider the sets $\mathcal{U}_n$ and $\mathcal{W}_n$ that contain all the n-dimensional subspaces of $\mathcal{U}$, resp. $\mathcal{W}$.

The *orthogonal complement* of such a finite dimensional subspace will be understood to be with respect to the $\mathcal{N}$-innerproduct; we exploit the following notation

$$\mathcal{U}_n^{\perp} = \{\ u \in \mathcal{U} \ \mid\ \mathcal{N}(u,v) = 0, \quad \textit{for all} \ \ v \in \mathcal{U}_n\ \},$$

resp.

$$\mathcal{W}_n^{\perp} = \{\ u \in \mathcal{W} \ \mid\ \mathcal{N}(u,v) = 0, \quad \textit{for all} \ \ v \in \mathcal{W}_n\ \}.$$

Theorem 86 *The eigenvalues λ_{n+1} are found from the following non-successive characterizations:*

- Weyl-Courant characterization

  $$\lambda_{n+1} = Max\ \left\{ Min\ \{\mathcal{R}(u) |\ u \in \mathcal{U} \cap \mathcal{W}_n^{\perp}\} \middle|\ \mathcal{W}_n \right\};$$

  the maximum is attained for the choice $\mathcal{W}_n = \mathrm{span}\{\varphi_1, \dots, \varphi_n\}$ (a set of n independent eigenfunctions with eigenvalue $\le \lambda_n$), and for that choice, the minimum is attained for an eigenfunction φ_{n+1} that has eigenvalue λ_{n+1};

- Poincaré characterization

  $$\lambda_{n+1} = Min\ \{Max\ \{\mathcal{R}(u) |\ u \in \mathcal{U}_{n+1}\} |\ \mathcal{U}_{n+1}\};$$

  the minimum is attained for the choice $\mathcal{U}_{n+1} = \mathrm{span}\{\varphi_1, \dots, \varphi_n, \varphi_{n+1}\}$ (a set of $n+1$ independent eigenfunctions with eigenvalue $\le \lambda_{n+1}$), and for that choice, the maximum is attained for an eigenfunction φ_{n+1} that has eigenvalue λ_{n+1}.

Proof.

- *Weyl-Courant*

  Let $\sigma = \mathrm{Max}\ \left\{ \{\mathrm{Min}\ \mathcal{R}(u) |\ u \in \mathcal{U} \cap \mathcal{W}_n^{\perp}\} \middle|\ \mathcal{W}_n \right\}$. For the choice $\mathcal{W}_n = span\{\varphi_1, \dots, \varphi_n\}$, it follows form the successive characterization that $\{\mathrm{Min}\ \mathcal{R}(u) |\ u \in \mathcal{U} \cap \mathcal{W}_n^{\perp}\} = \lambda_{n+1}$; hence $\sigma \ge \lambda_{n+1}$.

  Remains to show that $\lambda_{n+1} \ge \sigma$, i.e. that

  $$\lambda_{n+1} \ge \mathrm{Min}\ \{\mathcal{R}(u) | u \in \mathcal{W}_n^{\perp}\}, \quad \textit{for all} \ \ \mathcal{W}_n.$$

For this it is sufficient to show that, for any $\mathcal{W}_n$, there exists

$$\bar{u} \in \mathcal{W}_n^{\perp} \quad \textit{such that} \;\; \mathcal{R}(\bar{u}) \leq \lambda_{n+1} \textit{ and } \; u \in \mathcal{U}.$$

We construct $\bar{u}$ as a linear combination of the first $n+1$ eigenfunctions: take

$$\bar{u} = \sum_{1}^{n+1} \alpha_k \varphi_k \in \mathcal{U}$$

and determine the coefficients $\alpha_1, \ldots, \alpha_{n+1}$ in such a way that $\bar{u} \in \mathcal{W}_n^{\perp}$ and $\mathcal{N}(\bar{u}) = 1$ (this is possible!). Then

$$\mathcal{R}(\bar{u}) = \mathcal{Q}(\bar{u}) = \sum_{1}^{n+1} \lambda_k \alpha_k^2 \leq \lambda_{n+1} \sum_{1}^{n+1} \alpha_k^2 = \lambda_{n+1},$$

which completes the proof.

- *Poincaré*
  Let μ =Min $\{\{\text{Max } \mathcal{R}(u) |\; u \in \mathcal{U}_{n+1}\} |\; \mathcal{U}_{n+1}\}$. For the choice $\mathcal{U}_{n+1} = \textit{span}\{\varphi_1, \ldots, \varphi_n, \varphi_{n+1}\}$ it follows from the successive characterization that $\{\text{Max } \mathcal{R}(u) |\; u \in \mathcal{U}_{n+1}\} = \lambda_{n+1}$ and hence $\mu \leq \lambda_{n+1}$. To show the reversed inequality, $\lambda_{n+1} \leq \mu$, it is necessary to show that

  $$\lambda_{n+1} \leq \{\text{Max } \mathcal{R}(u) |\; u \in \mathcal{U}_{n+1}\} \quad \textit{for all } \; \mathcal{U}_{n+1},$$

  and for this that, for any given $\mathcal{U}_{n+1}$ there exists $\bar{u}$ such that

  $$\bar{u} \in \mathcal{U}_{n+1}, \quad \lambda_{n+1} \leq \mathcal{R}(\bar{u}).$$

  When $\mathcal{U}_{n+1} = \textit{span}\{\varphi_1, \ldots, \varphi_n, \varphi_{n+1}\}$, the choice $\bar{u} = \varphi_{n+1}$ will do. In the other case, the set $\mathcal{U}_{n+1}$ will contain at least one element $\bar{u} \neq 0$ that can be choosen to be perpendicular to the first $n+1$ eigenfunctions: $\mathcal{N}(\bar{u}, \varphi_k) = 0$ for $1 \leq k \leq n+1$. From the successive characterization it then follows that $\mathcal{R}(\bar{u}) \geq \lambda_{n+2}$, and so $\mathcal{R}(\bar{u}) \geq \lambda_{n+1}$, which completes the proof. □

6.4.2 Comparison of non-principal eigenvalues

Using the non-successive characterizations, one can obtain comparison results in much the same way as for principal eigenvalues. We only treat the genearization of Proposition RefpropcompPrincEV.

Proposition 87 *Let $\mathcal{U}$ be the linear space, and $\mathcal{R}$ the Rayleigh quotient, and let theieigenvalues be found from the Weyl-Courant or the Poincaré characterization.*

Suppose that the eigenvalues λ_n *satusfy the successive characterization described in Theorem RefthmEVPsucc. Making the dependence on* $\mathcal{R},\mathcal{U}$ *explicit, write*

$$\lambda_n = \lambda_n(\mathcal{R},\mathcal{U})$$

Then each eigenvalue λ_n *depends monotononically on* $\mathcal{R}$ *and on* $\mathcal{U}$ *in the following senses:*

- $\lambda_n(\mathcal{R}_1,\mathcal{U}) \leq \lambda_n(\mathcal{R}_2,\mathcal{U})$ if $\mathcal{R}_1(u) \leq \mathcal{R}_2(u)$ for all $u \in \mathcal{U}$
- $\lambda_n(\mathcal{R},\mathcal{U}_1) \leq \lambda_n(\mathcal{R},\mathcal{U}_2)$ if $\mathcal{U}_1 \supset \mathcal{U}_2$.

Proof. The monotone dependence on $\mathcal{R}$ is proved with the Weyl-Courant characterization as follows. From

$$\mathcal{R}_1(u) \leq \mathcal{R}_2(u) \quad \textit{for all} \quad u \in \mathcal{U}$$

it follows for any set $\mathcal{W}_n$ that

$$\text{Min } \{\mathcal{R}_1(u)|u \in \mathcal{U} \cap \mathcal{W}_n^\perp\} \leq \text{Min } \{\mathcal{R}_2(u)|u \in \mathcal{U} \cap \mathcal{W}_n^\perp\},$$

and hence, for any set $\mathcal{W}_n$,

$$\text{Min } \{\mathcal{R}_1(u)|\ u \in \mathcal{U} \cap \mathcal{W}_n^\perp\} \leq \text{Max } \left\{\text{Min } \{\mathcal{R}_2(u)|\ u \in \mathcal{U} \cap \mathcal{W}_n^\perp\}\right|\ \mathcal{W}_n\}$$

and thus

$$\begin{aligned} &\text{Max } \left\{\text{Min } \{\mathcal{R}_1(u)|\ u \in \mathcal{U} \cap \mathcal{W}_n^\perp\}\right|\ \mathcal{W}_n\} \\ &\quad\leq\quad \text{Max } \left\{\text{Min } \{\mathcal{R}_2(u)|\ u \in \mathcal{U} \cap \mathcal{W}_n^\perp\}\right|\ \mathcal{W}_n\} \end{aligned}$$

which shows that $\lambda_{n+1}(\mathcal{R}_1,\mathcal{U}) \leq \lambda_{n+1}(\mathcal{R}_2,\mathcal{U})$.
The monotone dependence on the domain is most easily proved with Weyl-Courant. To that end, let $\mathcal{W}_n$ be n-dimensional subsets of the largest (!) space $\mathcal{U}_1$. Then, since $\mathcal{U}_1 \cap \mathcal{W}_n^\perp \supset \mathcal{U}_2 \cap \mathcal{W}_n^\perp$,

$$\text{Min } \{\mathcal{R}(u)|u \in \mathcal{U}_1 \cap \mathcal{W}_n^\perp\} \leq \text{Min } \{\mathcal{R}(u)|u \in \mathcal{U}_2 \cap \mathcal{W}_n^\perp\},$$

and hence, for any set $\mathcal{W}_n$,

$$\text{Min } \{\mathcal{R}(u)|\ u \in \mathcal{U}_1 \cap \mathcal{W}_n^\perp\} \leq \text{Max } \left\{\text{Min } \{\mathcal{R}(u)|\ u \in \mathcal{U}_2 \cap \mathcal{W}_n^\perp\}\right|\ \mathcal{W}_n\}$$

and thus

$$\begin{aligned} &\text{Max } \left\{\text{Min } \{\mathcal{R}(u)|\ u \in \mathcal{U}_1 \cap \mathcal{W}_n^\perp\}\right|\ \mathcal{W}_n\} \\ &\quad\leq\quad \text{Max } \left\{\text{Min } \{\mathcal{R}(u)|\ u \in \mathcal{U}_2 \cap \mathcal{W}_n^\perp\}\right|\ \mathcal{W}_n\} \end{aligned}$$

which shows that $\lambda_{n+1}(\mathcal{R},\mathcal{U}_1) \leq \lambda_{n+1}(\mathcal{R},\mathcal{U}_2)$. $\square$.

Exercise 88 *1.* Provide the proof of the monotone dependence of the eigenvalues on R by using the Poincaré characterization.

2. Referring to Ex. 84, show that the results obtained there for the principal eigenvalue also hold for the other eigenvalues.

6.5 Exercises

1. *Poincaré-type of estimates*
   For functions $u \in C^1([0,1])$ the following *Poincaré (-Friedrichs-Wirtinger) inequalities* inequalities hold for suitable constants c_1, c_2, c_3:

   $$|u|_\infty^2 \leq c_1 \int_0^1 u_x^2$$

   $$\int_0^1 u^2 \leq c_2 \int_0^1 u_x^2$$

   $$|u|_\infty^2 \leq c_3 \int_0^1 u_x^2$$

   (a) Prove the inequalities.

   (b) Show that for functions on $[0,\infty]$ there is a constant c_4 such that

   $$\int_0^\infty [u^2 + u_x^2]dx \geq c_4 u(0)^2.$$

   (c) Note that the problem to find the "best" constants in the inequalities above is a variational problem itself. Determine, if possible, the best possible constant, and the function for which it is attained.

   (d) Now consider a domain $\Omega \in \mathcal{R}^n$; Ω may be unbounded, but suppose that at least in one direction it is bounded; specifically, say that for some $M > 0, |x_1| \leq M$ for all $x = (x_1, \dots, x_n) \in \Omega$. Show that for a constant c_5 it holds that all functions that satisfy $u = 0$ on (the finite part of) the boundary $\partial\Omega$:

   $$\int_\Omega u^2 dx \leq c_5 \int_\Omega |\nabla u|^2 dx.$$

2. *Eigenvalue problems, examples*

   (a) Proof with the methods of this chapter that the EVP from Linear Algebra

   $$Ax = \lambda Bx,$$

   with A and $B > 0$ symmetric matrices, has a complete set of eigenvectors.

   (b) Study the EVP for the Laplace operator with *Neumann* boundary conditions for a domain $\Omega \in \mathcal{R}^2$ in case

   - Ω is the rectangle $[0,a] \times [0,b]$,
   - Ω is the unit disc.

(c) Consider the EVP for the quadratic forms (corresponding to the bar-problem)

$$\mathcal{Q}(u) = \int_0^\ell u_{xx}^2, \quad \mathcal{N}(u) = \int_0^\ell u^2,$$

on each of the following sets:

$$\mathcal{U}_1 = \{ \ u \in C^2([0,\ell]) \ \mid \ u(0) = u(\ell) = 0 \ \},$$

$$\mathcal{U}_2 = \{ \ u \in C^2([0,\ell]) \ \mid \ u(0) = u_x(0) = u(\ell) = u_x(\ell) = 0 \ \}.$$

- Determine the eigenvalues and -functions explicitly; verify that the dependence on domain, and on the boundary conditions are in agreement with the general theory of this chapter.
- To investigate the corresponding inhomogeneous BVP
  $$\partial_x^4 u = f(x),$$
  for given function f, with the boundary values correponding to the variational formulation on the sets above, write down the inverse (integral) operator with the aid of Greens function in terms of the eigenvalues and -functions found.
- Derive a comparison result for the eigenvalues of $\mathcal{Q}$ on $\mathcal{U}_1$ and those of $\int u_x^2$ on the same set (and the same $\mathcal{N}$).
- Is it possible to compare the eigenvalues of $\mathcal{Q}$ on $\mathcal{U}_2$ with those of $\int u_x^2$ on the set $\mathcal{U}_1$?

3. Consider the vibrations of a square membrane, $(x,y) \in [0,\pi]^2$, that is fixed at the boundaries. The governing equation reads:

$$\partial_t^2 u(x,y,t) = \text{ div } (\sigma \nabla u) \tag{6.1}$$

where σ is a positive function depending on material properties. Solutions of the form

$$u(x,y,) = \sin(\omega t) v(x,y)$$

are called time harmonic vibrations, with frequency ω, and spatial deflection $v(x,y)$

(a) Determine the equation for $v(x,y)$, and a corresponding constrained variational formulation.

(b) Determine for the case $\sigma(x,y) = 1$ the possible frequencies and the corresponding spatial deflections.

(c) For $\sigma(x,y) = 5 + \sin(x)\cos(y)$, determine lower and upper bounds for each of the possible frequencies. (Do not try to calculate these values explicitly.)

4. *Transformation of 1D Sturm-Liouville operators*

(a) Consider a general operator $L = a(x)\partial_x^2 + b(x)\partial_x + c(x)$; unless specific conditions on the functions a and b are satisfied, this operator is not symmetric. Find a transformation $u(x) \to v(x)$ of the from

$$u(x) = g(x)v(x)$$

such that for suitably choosen function $g(x)$ the equation $Lu = f(x)$ transforms to $L_s v = h(x)$, where L_s is a symmetric operator. Hence, upon a suitable transformation, *any second order differential operator in one variable can be transformed to a symmetric operator to which variational techniques can be applied.*

(b) Consider on the interval $[0, \pi]$ the EVP for the S-L-operator

$$\partial_x p(x)\partial_x u(x) + q(x)u(x) = \lambda\rho(x)u(x), \quad x \in (0, \pi),$$

with p, ρ strictly positive functions. Show that under the transformation

$$u(x) \to v(t), \quad v = (p\rho)^{\frac{1}{4}}u, \ t = \int_0^x \sqrt{\frac{\rho}{p}}, \ \ (\ell = \int_0^\pi \sqrt{\frac{\rho}{p}})$$

the following equation for v results:

$$-\partial_t^2 v(t) + r(t)v(t) = \lambda v(t), \quad t \in (0, \ell)$$

for suitable function r. (Hence, in a S-L EVP, the function p can be “transformed away” to a constant).

5. *Nodal properties of solutions of Sturm-Liouville equations*

(a) Consider the S-L operator

$$L \equiv \partial_x p \partial_x + q$$

on an interval where $p > 0$. Let u be any nontrivial solution. Show that any zero of u (if any) is simple.

Proposition 89 *Any eigenvalue of the S-L-operator (with Dirichlet, Neumann or mixed boundary conditions) is simple: the corresponding eigenspace is one-dimensional.*

Prove this result.

(b) Consider two S-L operators

$$L_1 \equiv \partial_x p_1 \partial_x + q_1, \quad L_2 \equiv \partial_x p_2 \partial_x + q_2,$$

where p_m, q_m are functions defined on a bounded or unbounded interval I. Suppose that one set dominates the other set on the interval I:

$$p_1(x) \geq p_2(x), \quad q_1(x) \geq q_2(x)$$

Consider two functions u and v that satisfy

$$L_1 u(x) = 0, \quad L_2 v(x) = 0.$$

Show that, between any two successive nodal values of u (assuming that there are two zeros) there exists at least one zero of v.
Consequently: if u has infinitely many zeros, then so has v, and the zeros of u and those of v are alternating.

6. **Bessel functions**

Solutions of the so-called *Bessel differential equation* for functions on $x \geq 0$

$$u_{xx} + \frac{1}{x}u_x + (1 - \frac{\nu^2}{x^2})u = 0 \quad (x > 0).$$

are the so-called Bessel functions of order ν. For $\nu \geq 0$, there is one solution that is finite at $x = 0$, denoted by $J_\nu u(x)$, and called the *Bessel function of the first kind*, of order ν; the other solution, ususally denoted by $Y_\nu u(x)$, is a *Bessel function of the second kind*, a solution that is singular at $x = 0$.
The Bessel function J_0 does not vanish at $x = 0$, and can be normalized to unity: $J_0(0) = 1$. On the other hand, $J_m(0) = 0$ for $m \geq 0$.
For $\nu = m$, with $m = 0, 1, \ldots$, the Bessel functions J_m are alternating and decay like $\frac{1}{\sqrt{x}}$; asymptotically, the "period" tends to a fixed number 2π, and so

$$J_m(x) \approx \sqrt{\frac{2}{\pi x}} \sin(x + \alpha_m)$$

where α_m is a certain constant.
The successive zeros of the Bessel function J_m are all simple and denoted by $\sigma_{m,\ell}, \ell \geq 1$; this sequence tend to infinity: $\sigma_{m,\ell} \to \infty$ as $\ell \to \infty$.

We will now investigate some of the properties mentioned above.

(a) *Transformation of Bessel equation, asymptotic behaviour*

- Show that the transformation (see above for the general theory)
$$v(x) = \sqrt{x}u(x)$$
leads to the following equation for v:
$$v_{xx} + r(x)v(x) = 0, \ \textit{with} \ \ r(x) = 1 + \frac{\frac{1}{4} - \nu^2}{x^2}$$
- Observe that when x tends to infinity, $r(x)$ tends to 1, so for large x the equation for v is approximately
$$u_{xx} + u = 0$$
with solutions $A\sin(x + \varphi)$. In order to fill in the words 'approximately'and 'large' one has to do some effort which is neatly described in for instance Olver (1974). But with the use of MAPLE we can get an idea of how well this shifted sine approximates our

Bessel functions. So, fill in the following table with the help of MAPLE:

$$\sqrt{x}J_m(x) \approx \sqrt{\frac{2}{\pi}}\sin(x+\alpha_m) \quad \textit{for} \quad x \to \infty$$

m	0	1	2	3
α_m				

(b) *Nodal properties of Bessel functions*
We observed that the Bessel functions kept alternating, i.e. they have infinitely many zeros. But we needed some asymptotics in order to come to this statement, and these approximations weren't even justified! Prove the following statement.

Proposition 90
(i) All zeros ($\neq 0$) of a solution of the Bessel differential equation are simple.
(ii) $J_\nu u(x)$ *has countable infinitely many positive zeros,* $\sigma_{\nu,\ell}$.
(iii) The distance between successive zeros of $J_\nu u(x)$ *is:*
$< \pi$ *when* $|\nu| < \frac{1}{2}$, $= \pi$ *when* $|\nu| = \frac{1}{2}$, *and* $> \pi$ *when* $|\nu| > \frac{1}{2}$.

Hint: Use the transformed differential equation for the Bessel functions obtained above to show that the Bessel functions have infinitely many zeros, and give the estimate for the spatial distance by comparing with the simple equations on IR

$$w_{xx}(x) + cw(x) = 0$$

for two suitably choosen constants c_1 and c_2.

(c) Compute with MAPLE the integral

$$\int_0^1 xJ_0(\sigma_{0,k}x)J_0(\sigma_{0,\ell}x)\,dx$$

for both $k \neq \ell$ and $k = \ell$.

7. *Non-linear boundary value problem*
Consider the nonlinear BVP

$$-u_{xx} = f(u), \quad u(0) = u(1) = 0.$$

This may be the equation for time-independent states of a *reaction-diffusion* equation for the concentration u (necessarily non-negative), and $f(u)$ a source due to reactions.
Let $\Lambda \equiv \pi^2$ be the principal eigenvalue of $-\partial_x^2$ for the given boundary conditions.

(a) Determine the variational formulation: the functional $\mathcal{L}(u)$ for which the critical points satisfy the equation.

(b) Show that if $u \neq 0$ is any non-trivial solution, then necessarily the function

$$x \to f(u(x)) - \Lambda u(x)$$

changes sign on $]0,1[$.

(c) Prove that if $f(0) = 0$ (then $u \equiv 0$ is a solution), and moreover

$$z[f(z) - \Lambda z] < 0 \quad \textit{for all} \ \ z \neq 0,$$

then $u \equiv 0$ is the *only* solution.

(d) Investigate, and interpret the results above, with phase-plane analysis.

(e) As a specific example, consider the BVP

$$-u_{xx} = \mu \sin u, \quad u(0) = u(1) = 0,$$

for $\mu \in IR$ (*Euler buckling*). Show that for $\mu \leq \Lambda$, the trivial solution is the only solution.
Show that the functional $\mathcal{L}(u) = \int [\frac{1}{2} u_x^2 - \mu(1 - \cos u)]$ has the following properties:

- For $\mu \leq \Lambda$ it holds that $\mathcal{L}(u) \geq 0$, and so $u \equiv 0$ provides the absolute minimum for $\mathcal{L}$.
- For $\mu > \Lambda$, the functional $\mathcal{L}$ can attain negative values.
- For $\mu > \Lambda$, $u \equiv 0$ is not the global minimizer for $\mathcal{L}$, nor is it a local minimizer (investigate the second variation).

(f) Investigate in the same way the functional for the more general BVP with $f(u)$.

Chapter 7

Convexity theory

7.1 Basic definitions and properties

In the following $\mathcal{U}$ is a linear space, finite or infinite dimensional; we use the notation for infinite dimensional spaces. In this section we recall the basic notions of convex sets and convex functionals, and the simplest properties of convex functionals.

7.1.1 Convex sets and convex functionals

For given elements $u, v \in \mathcal{U}$, and $\sigma \in [0,1]$, we will call $\sigma u + (1-\sigma)v$ the *convex combination*; for shortness we will write this as $\sigma u + \sigma^* v$.

Definition 91 *A set $\mathcal{C} \subset \mathcal{U}$ is called a* convex set *if with each two points in $\mathcal{C}$ any convex combination belongs to $\mathcal{C}$:*

$$\forall u, v \in \mathcal{C} \ \forall \sigma \in [0,1] \quad \sigma u + \sigma^* v \in \mathcal{C}.$$

Equivalently: the whole line between u and v belongs to $\mathcal{C}$.

Exercise 92 *1.* A linear space is convex, and so is any linear subspace.

2. The following set is a convex subset of $C^0([0,1])$ for any given pair of continuous functions φ and ψ*:*

$$\mathcal{C} = \{ \ u \in C^0([0,1]) \ \mid \ \varphi(x) \leq u(x) \leq \psi(x) \ \text{ for all } \ x \in [0,1] \ \}.$$

Definition 93 *A functional F defined on a convex set is called a* convex functional *if its value at a convex combination is dominated by the convex combination of the values*

$$\forall u, v \in \mathcal{C} \ \forall \sigma \in [0,1] \quad F(\sigma u + \sigma^* v) \leq \sigma F(u) + \sigma^* F(v);$$

the functional is called stictly convex *if equality holds only in the trivial cases:*

$$\forall u, v \in \mathcal{C} \ , u \neq v \ \forall \sigma \in]0,1[\quad F(\sigma u + \sigma^* v) < \sigma F(u) + \sigma^* F(v).$$

A functional G is called a (strictly) concave functional *if $-G$ is (strictly) convex.*

Convex functions on an interval are clearly characterized by the property of their graph. But so is a convex functional, since from the definition it readily follows that *a functional F is convex on $\mathcal{C}$ iff F is a convex function on each line interval belonging to C.*

There is a simple relation between convex sets and convex functionals by using the notion of epigraph.

Definition 94 *For given functional $F: \mathcal{C} \to IR$, the* epigraph *of the functional F is the set in the product space $\mathcal{U} \times IR$ defined by*

$$epi(F) := \{ \ (u, \tau) \in \mathcal{C} \times \mathcal{R} \ \mid \ F(u) \leq \tau \ \}.$$

Proposition 95 *The functional F is convex on the set $\mathcal{C}$ iff its epigraph is a convex set in $\mathcal{U} \times \mathcal{R}$.*

Exercise 96

1. Any linear functional is convex, but not strictly convex.
2. The level sets of a functional are convex sets iff the functional is a linear functional.
3. Let $f: R \to R$ be a convex function, and $U = C^0(\Omega)$. Then the functional
$$F(u) := \int_\Omega f(u(x))dx,$$
a so-called *substitution functional,* or *Nemytski functional,* is convex.
4. More generally, if for every $x \in \Omega$ the function $f(x, \cdot): R \to R$ is convex, then the functional
$$F(u) := \int_\Omega f(x, u(x))dx,$$
is convex.
5. Show that on $U = \{u : \Omega \to R \ \mid \ u(x) = \varphi(x) \ on \partial\Omega \ \}$ the following functionals are convex
$$\int_\Omega |\nabla u|^2, \quad \int_\Omega (\Delta u)^2,$$
and so is the Sturm-Liouville form for positive functions p, q:
$$\int_\Omega [p(x)|\nabla u|^2 + q(x)u^2].$$

6. For a finite number of points $\{u_1, \dots, u_N)\}$ a *convex combination* is by definition any linear combination of the form

$$\sum \alpha_k u_k, \text{ with } \alpha_k \geq 0, \quad \sum \alpha_k = 1.$$

Show that convexity of a function F implies that for any convex combination

$$F(\sum \alpha_k u_k) \leq \sum \alpha_k F(u_k).$$

Proposition 97 *Let $f : \mathcal{R} \to \mathcal{R}$ be a convex function, and $u : [0,1] \to \mathcal{R}$ an integrable function. Then the following inequality holds:*

$$f\left(\int_0^1 u(x)dx\right) \leq \int_0^1 f(u(x))dx.$$

7. Prove this result in two ways. First, in a limiting process, replace the integral with a Riemann sum, and use the result above about convex combinations. Secondly, assuming that f is twice differentiable, by observing that (with $\bar{u} = \int_0^1 u(x)dx$, and $xi(x)$ a suitable function)

$$\int_0^1 [f(u(x)) - f(\bar{u})]dx$$

$$= \int_0^1 [f'(\bar{u})(u(x) - \bar{u})]dx + \int_0^1 [f''(xi(x))(u(x) - \bar{u})^2]dx \geq 0.$$

8. In the inequality above one should be careful with the scaling-property:

Proposition 98 *Let $f : IR \to IR$ be a convex function, and $u : \Omega \to IR$ an integrable function. Then the following inequality holds;*

$$f\left(1/|\Omega| \int_\Omega u(x)dx\right) \leq \frac{1}{|\Omega|}\int_\Omega f(u(x))dx, \text{ with } |\Omega| = \int_\Omega dx.$$

As a consequence, for integrable functions u:

$$\left|\int_0^1 u(x)dx\right|^\alpha \leq \int_0^1 |u(x)|^\alpha dx, \quad \text{for } \alpha > 1.$$

and

$$\left|\int_a^b u(x)dx\right|^\alpha \leq (b-a)^{(\alpha-1)} \int_a^b |u(x)|^\alpha dx, \quad \text{for } \alpha > 1.$$

7.1.2 Differentiable convex functionals

Recall the properties of a differentiable function of one variable:

$$\begin{aligned} f : IR \to IR \text{ is convex iff} \quad & f' \text{ is monotonically non-decreasing,} \\ \text{i.e. iff} \quad & f'' \geq 0. \end{aligned}$$

The same holds true more generally. Using the notation for first and second variation, we have

Proposition 99 *If F is convex on $\mathcal{C}$, the following holds for all $u, v \in \mathcal{C}$:*

1. $F(v) - F(u) \geq \delta F(u; v - u)$*;*
2. $\delta F(u; u - v) - \delta F(v; u - v) \geq 0$*;*
3. $\delta^2 F(u; v - u) \geq 0$*.*

Proof.

1. From the convexity it follows that for any $\sigma \in [0, 1]$

   $$F(\sigma u + \sigma^* v) - F(u) \leq \sigma[F(v) - F(u)];$$

   deviding by σ and taking the limit $\sigma \to 0$ leads to the result.
   An alternative proof is by noting that $f(\sigma) := F(\sigma u + \sigma^* v)$ is a convex function of the scalar variable σ. Since $f(1) - f(0) \geq f'(0)$, the result is immediate.

2. Adding $F(v) - F(u) \geq \delta F(u; v - u)$ and $F(u) - F(v) \geq \delta F(v; u - v)$ (role of u and v interchanged), the result follows.

3. For $f(\sigma) := F(\sigma u + \sigma^* v)$ it holds that $f''(1) \geq 0$, and hence the result since $f''(1) = \delta^2 F(u; v - u)$. □

7.2 Convex minimization problems

7.2.1 Minimizers are unique or form a convex set

Proposition 100 *The minimizers of a convex functional F on a convex set $\mathcal{C}$ form a convex subset (possibly empty); when F is strictly convex, there is at most one minimizer.*

Proof. If the infimum

$$\mu = \inf \{F(u) | \; u \in \mathcal{C}\}$$

is attained for two minimizers, say $\hat{u}$ and $\hat{v}$, then so the infimum is attained for any convex combination:

$$\mu \leq F(\sigma \hat{u} + \sigma^* \hat{v}) \leq \sigma F(\hat{u}) + \sigma^* F(\hat{v}) = \sigma\mu + \sigma^* \mu = \mu,$$

which proves the fact that the set of minimizers is a convex set (when non-empty). When stricly convex, $\mu = F(\hat{u}) = F(\hat{v})$ implies $\hat{u} = \hat{v}$. □

Exercise 101 *1.* The following set of nonlinear algebraic equations has a unique solution:

$$\begin{cases} 4x^3 + 2xy^2 + 2x & = 7, \\ 3y^5 + x^2 y & = -3. \end{cases}$$

2. From the variational formulation it follows that the solution of the BVP

$$\begin{cases} -\Delta u & = f(x) & \text{in}\Omega, \\ u(x) & = \varphi(x) & \text{on}\partial\Omega_1, \\ \partial_n u(x) & = \psi(x) & \text{on}\partial\Omega_2 \end{cases}$$

is unique for every choice of functions f, φ, ψ.

3. Show that when the potential energy is *concave* (instead of convex, as is usually the case), the second order Hamiltonian system

$$-\ddot{q} = V'(q)$$

has at most one T-periodic solution.

4. Give a sufficient condition for the function $f = f(x, u)$ that assures that the solution of the BVP

$$\begin{cases} -\Delta u & = f(x,u) & \text{in } \ \Omega, \\ u(x) & = \varphi(x) & \text{on } \ \partial\Omega_1, \\ \partial_n u(x) & = \psi(x) & \text{on } \ \partial\Omega_2 \end{cases}$$

is unique for every choice of functions φ, ψ.
Consequently, for $\varphi = \psi \equiv 0$ and $f(x, 0) = 0$, the only solution is the trivial solution.

5. Show that the trivial solution is the only solution of

$$\begin{cases} \Delta u & = u^3 & \text{in } \ \Omega, \\ u(x) & = 0 & \text{on } \ \partial\Omega. \end{cases}$$

(Use the results above; give also a direct proof by taking the innerproduct of the equation with u.)

7.2.2 Variational inequalities

To motivate, and prepare for, the following more general result, consider a differentiable function on a finite interval $f : [a, b] \to \mathcal{R}$. Suppose f attains its minimum on the interval at the point $\hat{x}$.
If f is convex, we have information about its derivative at $\hat{x}$, even if $\hat{x}$ is a boundary point:

$$\begin{array}{ll} f'(\hat{x}) = 0 & \textit{if } \hat{x} \in]a, b[, \\ f'(\hat{x}) \geq 0 & \textit{if } \hat{x} = a, \\ f'(\hat{x}) \leq 0 & \textit{if } \hat{x} = b. \end{array}$$

Taken together, this can be stated like

$$f'(\hat{x}).(x - \hat{x}) \geq 0, \quad \textit{for all } x \in [a, b].$$

This is an example of a variational inequality; it replaces Fermat's algorithm for convex functions to allow that the extremum is achieved at the boundary.
We will now generalize this result.

Proposition 102 *For a convex set $\mathcal{C}$ and convex functional F, let $\hat{u}$ be the minimizer:*

$$\hat{u} \in \textit{inf } \{F(u) |\ u \in \mathcal{C}\}.$$

The $\hat{u}$ satisfies the following variational inequality*:*

$$\delta F(\hat{u}; v - \hat{u}) \geq 0 \ \text{ for all } \ v \in \mathcal{C}.$$

Proof. For every $v \in \mathcal{C}$, the function $f : [0, 1] \to I\!R$, defined by $f(\sigma) := F(\hat{u} + \sigma(v - u))$ is convex and attains its minimum at $\sigma = 0$; hence $f'(0) \geq 0$, and the result follows since $f'(0) = \delta F(\hat{u}; v - \hat{u})$. □

Exercise 103 *1. Fermat's algorithm.*
When $\hat{u} \in C \subset U$ is an *interior point*, the variational inequality implies Fermat's algorithm: $\delta F(\hat{u}; \eta) = 0$ for all $\eta \in U$.

2. Linear multiplier rule
When C is a level set of a linear functional, say $C = \{\ u \ \mid\ \ell(u) = c\ \}$, the variational inequality implies $\delta F(\hat{u}; \eta) = 0$ for all η for which $\ell(\eta) = 0$; Lagrange's (linear) multiplier rule then leads to $\delta F(\hat{u}; v) = \lambda \ell(v)$ for all $v \in U$.

Exercise 104 Let ψ be a given concave function on $[0, 1]$, that is positive somewhere, but $\psi(0) < 0, \psi(1) < 0$.
We look for the shortest "distance" from $(0, 0)$ to $(1, 0)$ when the graph of ψ acts like a barrier:

$$\textit{inf } \left\{ \int_0^1 u_x^2 dx \middle|\ u(0) = u(1) = 0; u(x) \geq \psi(x) \right\}.$$

1. Verify that the variational inequality in this case reads

$$\int_0^1 u_x(v_x - u_x)dx \geq 0, \quad \text{for all} \quad v \geq \psi.$$

2. Define the sets where a function coincides with or is free of the barrier:

$$\begin{array}{lcl} \Gamma_- & := & \{\ x \in]0,1[\ \mid\ u(x) = \psi(x)\ \}, \\ \Gamma_+ & := & \{\ x \in [0,1]\ \mid\ u(x) > \psi(x)\ \}. \end{array}$$

   Interpret these sets geometrically; convince yourself that it is plausible that, since ψ is concave, the sets consists of intervals: for a, b the *free boundary points*:

$$\Gamma_- = [a,b] \subset [0,1], \quad \Gamma_+ = [0,a] \cup [b,1].$$

3. Show that at points $x \in \Gamma_+$ the minimizer will satisfy $u_{xx} = 0$ in a neighbourhood.

4. Determine candidate-minimizers from the two observations above, with a, b still to be determined.

5. Calculate the functional on the candidate-minimizers, and find a function of the free boundary points, say $F(a,b)$.

6. Find the optimal value of the functional from

$$inF(a,b)a,b.$$

7. Determine the corresponding extremal, and show that it satisfies at the boundary points

$$u_x(a) = \psi_x(a), \quad u_x(b) = \psi_x(b).$$

8. Observe that the optimal solution found in this way is in fact a differentiable function on the whole interval $[0,1]$.

7.3 Duality: Legendre (-Fenchel) transformation

In this section we deal with one of the most important aspects of convex functions. It states that a convex functional can be described as the envelope of a family of linear functionals; this is intuitively clear when one looks at the graph of a function of one variable, and takes the family of tangent lines at each point of the graph. The same approach can be used to define a more general convex set. Compared to the foregoing, the previous definitions defined convex sets and convex functions “from the interior" (with any two interior points the connecting straight line belongs to the set or epigraph). The results to follow

show that they characterize convex functions “from the outside".
We start with the standard Legendre transformation, requiring strong conditions on the functional. Then we relax the conditions and describe the corresponding so-called Fenchel transformation. As an important byproduct we get Young’s inequality.

7.3.1 Supporting lines and hyperplanes to convex functions

For a differentiable function $f : \mathcal{R} \to \mathcal{R}$ the tangent line at a point $\hat{x}$ is given by

$$x \to \ell(x) := f(\hat{x}) + f'(\hat{x})(x - \hat{x}).$$

This line devides the plane $\mathcal{R} \times \mathcal{R}$ in two half planes:the upper half plane $\{x \mid \ell(x) > 0\}$ and the lower half plane $\{x \mid \ell(x) < 0\}$. If f is a convex function, its graph is on one side, in the upper half plane:

$$f(x) \geq \ell(x) \quad \textit{for all} \quad x;$$

the tangent line ”supports” the graph at the point $\hat{x}$.
Observe that, given the tangent direction $\mu := f'(\hat{x})$, ℓ is the maximal function with the property that the graph of f lies in the upper half plane. In formulas: for $\alpha \in \mathcal{R}$

$$x \mapsto \ell_\mu(x) := \mu x - \alpha$$

it holds that

$$f(x) \geq \ell_\mu(x) \quad \textit{iff} \quad \alpha \geq \alpha^*,$$

where

$$\alpha^* = \mu\hat{x} - f(\hat{x}).$$

This lower bound for α clearly depends on μ and can be equivalently characterized as

$$\alpha^* \equiv \sup_x [\mu x - f(x)]$$

which defines a function $\alpha^* \equiv f^*(\mu)$, the socalled dual function of f. This transformation from a function to its dual is a transformation in the description of the graph of the function by point values and by a family of supporting tangent lines. Under suitable conditions we will see below that these descriptions are equivalent for convex functions.

7.3.2 Dual function and Legendre transform

The construction of supporting tangent lines to a convex function can be generalized in a straigthforward way as follows.
Let $\mathcal{U}$ be a function space, with dual space $\mathcal{U}^*$; the duality map will be denoted by $\langle \ , \ \rangle$. In our examples this will be the L_2-innerproduct.
Given $u^* \in \mathcal{U}^*$, consider the linear functional for $\alpha \in I\!R$

$$\ell_\mu(u) := \langle u^*, u\rangle - \alpha.$$

Then the zero level set of ℓ_μ defines a hyperplane (codimension 1) that separates the upper and lower half spaces.

Definition 105 *For given functional $F : \mathcal{U} \to I\!R$, the dual functional F^* is defined on $\mathcal{U}^*$, possibly with values in $I\bar{R} \equiv I\!R \cup \{+\infty\}$, by*

$$F^*(u^*) := \sup_{u\in\mathcal{U}} [\langle u^*, u\rangle - F(u)].$$

A first property of this dual functional is that it is convex.

Proposition 106 *For any functional F its dual functional (with values in $I\bar{R}$) is convex.*

Since $u^* \mapsto \langle u^*, u\rangle - F(u)$ is for each $u \in \mathcal{U}$ a linear, and hence a convex, functional, the result is an easy consequence of the following Lemma.

Lemma 107 *Given any function of two variables $f(u,x)$ that is convex in x for every u, the function*

$$g(x) := \sup_u f(u,x)$$

is convex (as a function in $I\bar{R}$).

Proof.
For a convex combination $\sigma x + \sigma^* y$ and any u it holds that

$$f(u, \sigma x + \sigma^* y) \le \sigma f(u,x) + \sigma^* f(u,y)$$

$$\le \sup_u [\sigma f(u,x)] + \sup_u [\sigma^* f(u,y)] = \sigma g(x) + \sigma^* g(y)$$

and hence, by taking the supremum over u of the first term

$$g(\sigma x + \sigma^* y) \le \sigma g(x) + \sigma^* g(y)$$

the convexity of g. □

Exercise 108 *Let $\mathcal{C}$ be a convex set in $I\!R^n$, bounded in some or all directions.*

1. Define the *polar function* of C as

$$\chi_{\mathcal{C}}(n) := \sup_{x\in\mathcal{C}}\langle n, x\rangle.$$

   Verify that this function is convex, and give a geometrical interpretation of this function.

2. Determine the dual function and show that it characterizes the set C.
3. Let F be a convex function. Relate the polar function (and its dual) of its epigraph with the (bi-) dual function of F.

Having defined the dual function in the above way, it is not necessary that the supremum is finite, nor that it is attained. Furthermore, it would be nice if the original function F could be recovered from the dual function (which can intuitively be expected when F is convex, make pictures). This can indeed be proved when F is convex. This is shown first for the case of functions that satisfy a Legendre condition; in the next subsection we generalize to more general functionals. When possible, the function F is found as the dual of the dual function. This leads one to introduce the following notion.

Definition 109 *The* bidual F^{**} *of a function* F *is defined as*

$$F^{**}:\mathcal{U}\equiv (U^*)^*\to IR,\quad F^{**}:=(F^*)^*.$$

Proposition 110 *Any function* F *dominates its bi-dual:*

$$F^{**}(u)\le F(u)\ \text{ for all }\ u\in\mathcal{U}$$

Proof. Directly from

$$F^{**}(u)=\sup_{u^*}[\langle u^*,u\rangle - F^*(u^*)]=\sup_{u^*}[\langle u^*,u\rangle - sup_v[\langle u^*,v\rangle - F(v)]]$$

$$=\sup_{u^*}\inf_{v}[\langle u^*,u-v\rangle + F(v)]\le \inf_{v}\sup_{u^*}[\langle u^*,u-v\rangle + F(v)]=F(u),$$

where we used the inequality that is valid for all functions $f(x,y)$:

$$\sup_x\inf_y f(x,y)\le\inf_y\sup_x f(x,y).$$

Definition 111 *The class of* Legendre functionals *on* $\mathcal{U}$ *(a reflexive Banch space) are functionals* F *that satisfy the following conditions:*

1. F *is* superlinear *at infinity, meaning*

$$\lim_{||u||\to\infty}\frac{F(u)}{||u||}\to\infty,$$

2. F *is strictly convex,*

3. *F is differentiable.*

Proposition 112 Legendre transformation
Let F be a Legendre functional on $\mathcal{U}$.

1. *In the defining expression for F^*, for each u^* the sup is attained at a unique point, and the expression reduces to the so-called* Legendre transformation
$$\begin{aligned} F^*(u^*) &= sup_u[\langle u^*, u\rangle - F(u)] \\ &\equiv \langle u^*, u\rangle - F(u) \quad \text{for} \quad u^* = \delta F(u). \end{aligned}$$
2. *The dual function F^* is a Legendre functional on $\mathcal{U}^*$.*
3. *The* bidual F^{**} *of F is the function F itself:*
$$F^{**}(u) = F(u).$$
4. *Consequently*
$$\begin{aligned} F(u) &= \sup_{u^*}[\langle u^*, u\rangle - F^*(u^*)] \\ &\equiv \langle u^*, u\rangle - F^*(u^*) \quad \text{for} \quad u = \delta F^*(u^*); \end{aligned}$$
5. *In particular, the derivatives are eachother inverse:*
$$u^* = \delta F(u) \Leftrightarrow u = \delta F^*(u^*).$$

Exercise 113 For given convex function f and its dual f^* the following inquality is a direct consequence of the definition of dual function:

$$f(x) + f^*(y) \geq xy \text{ forall} x, y$$

and

$$f(x) + f^*(y) = xy \text{ iff} y = f'(x), \quad x = (f^*)'(y).$$

In specific cases this inequality is known as Young's inequality. Verify the following special cases.

1. $e^x + y(\log y - 1) \geq xy$;
2. $x \log x - e^{y+1} \geq xy$;
3. for $\alpha > 1$ and $1/\alpha + 1/\beta = 1$:
$$\frac{1}{\alpha}x^\alpha + \frac{1}{\beta}y^\beta \geq xy.$$

7.3.3 Fenchel transformation

The following is a generalization of the Legendre transformation; strict convexity is not needed, nor differentiability. The condition on the semi-continuity place only a role on the "boundary" where F can take infinite values, as shown in the examples.

Proposition 114 *Let F be a convex functional that is lower semi-continuous. Then its bidual coincides with F: $F^{**} = F$. At points where F is not strictly convex, F^* has a discontinuous derivative; where F has discontinuous derivative, F^* is not strictly convex.*

Exercise 115 *1.* Let the function f be defined by

$$f(x) = \begin{cases} \frac{1}{2}x^2 & \text{for } |x| < 1, \\ \infty & \text{else} \end{cases}$$

Determine the dual function; investigate if $f^{**} = f$.

2. The same questions for the function

$$f_1(x) = \begin{cases} \frac{1}{2}x^2 & \text{for } |x| \leq 1, \\ \infty & \text{else} \end{cases}$$

3. Determine the dual and bidual function of

$$f(x) = |x|.$$

4. Determine the dual and bidual function of

$$f(x) = x^4 - x^2.$$

5. Determine the dual function of

$$f(v) = \sqrt{1 + v^2};$$

determine the dual functional of the length functional

$$F(u) = \int f(u_x)dx$$

7.4 Applications in Classical Mechanics

7.4.1 Lagrange and Hamilton equations

Consider a Lagrangian system with Lagrangian on configuration space $\mathcal{Q}$, i.e. $L = L(u, v; t), u \in \mathcal{Q}, v \in T_u\mathcal{Q}$, for which the evolution equation is given by

$$\frac{\partial}{\partial t}\delta_v L(u, \partial_t u; t) - \delta_u L(u, \partial_t u; t) = 0,$$

which is the Euler -Lagrange equation of the action functional

$$\mathcal{A}(u) = \int L(u, \partial_t u; t) dt.$$

Suppose that for each $u \in \mathcal{Q}, t \in IR$

$$v \to L(u, v; t)$$

is a Legendre functional. Define its dual function to be

$$H : T^*\mathcal{Q} \times IR : \ H(u, p; t) = \sup_v [\langle p, v\rangle - L(u, v; t)],$$

i.e. the Legendre transformation:

$$H(u, p; t) = \langle p, v\rangle - L(u, v; t) \quad \textit{for} \quad p = \delta_v L(u, v; t).$$

Then, equivalently,

$$\begin{aligned} L(u, v; t) &= \sup\nolimits_p [\langle p, v\rangle - H(u, p; t)] \\ &= \langle p, v\rangle - H(u, p; t) \ \ \textit{for} \quad v = \delta_p H(u, p; t). \end{aligned}$$

Inserting this in the action functional leads to the canonical action functional:

$$\begin{aligned} \mathcal{A}(u) &= \textstyle\int \sup_p [\langle p, v\rangle - H(u, p; t)] dt \\ &= \sup\nolimits_{p(t)} \textstyle\int [\langle p, v\rangle - H(u, p; t)] dt \equiv \sup_p \mathcal{CA}(u, p). \end{aligned}$$

This leads directly to the following result.

Proposition 116 *A Lagrangian system with Lagrangian on configuration space $\mathcal{Q}$ that is a Legendre function in the velocity variable v is equivalent to the Hamiltonian system on the cotangent space $T^*\mathcal{Q}$ as phase space and Hamiltonian the Legendre transform of the Lagrangian L.*

Proof. From the above observation the result follows directly from

$$\mathrm{Crit}_u \mathcal{A}(u) = \mathrm{Crit}_{u,p} \mathcal{CA}(u, p).$$

Hence the Lagrangian equations are equivalent to Hamiltons equations

$$\begin{cases} \partial_t u &= \delta_p H(u, p; t), \\ \partial_t p &= -\delta_p H(u, p; t) \end{cases}$$

□

The reverse of the above also holds.

Proposition 117 *A Hamiltonian sytem on a cotangent space $T^*\mathcal{Q}$ with Hamiltonian that is a Legendre function in the momentum variable is equivalent to the Lagrangian system on the configuration space $\mathcal{Q}$ with Lagrangian that is the Legendre transform of the Hamiltonian.*

Exercise 118 *1.* Prove the two Propositions above by showing directly from the equations that the Lagrange equations transform to Hamiltons equations under the Legendre transformation, and visa versa. Note that this is a more complicated way then by using the functionals.

2. ***Energy conservation***
When for the Hamiltonian system the Hamiltonian does not depend explicitly on time, H is conserved. After Legendre transformation this correspond precisely with the energy conservation in terms of the Lagrangian (which also does not depend on time explicitly), as described earlier:

$$\frac{d}{dt}H(q,p) = 0 \Leftrightarrow \frac{d}{dt}[\dot{q}\partial_v L(q,\dot{q}) - L(q,\dot{q})] = 0.$$

3. Give the Hamiltonian formulation (canonical variables, Hamiltonian and Hamiltons equations) of the following Lagrangian systems:

(a) $$-\partial_t^2 q = \partial_q V(q), \quad q \in IR^N;$$

(b)

$$\partial_t^2 u = u_{xx} + f(u);$$

(c) The motion of a mass point in the plane under the influence of a conservative force (potential V) in Cartesian and in polar coordinates; derive the description in polar coordinates by first transforming the Lagrangian to polar coordinates and then the Hamiltonian by a Legendre transformation.

(d) Give the Hamiltonian formulation for geodesic problems described by a length functional

$$\mathcal{L}(u) = \int n(x,u)\sqrt{1+u_x^2}dx.$$

7.4.2 Hamilton-Jacobi theory

Consider a given finite dimensional Lagrangian system with Lagrangian $L(q,v)$. For a given initial point (t_0, q_0), suppose that for any (T,Q) in a neighbourhood there exists a unique extremal through the two points. This means that there is a *family of extremals*.
Consider the corresponding value function as a function of the end point:

$$S(T,Q) = \text{Crit} \left\{ \int_{t_0}^{T} L(q,\dot{q})dt \,\middle|\, q(t_0) = q_0; q(T) = Q \right\}.$$

Observe that a levelset of S, say $S(T,Q) = \sigma$, can be interpreted as the points that are at a distance σ from (t_0, q_0), the distance being measured with the value of the action functional.

Exercise 119 *1.* For geodesic problems in the plane, with extremals as the graph of functions of x, level sets of the corresponding value function

$$S(X,Y) = Crit \left\{ \int_{x_0}^{X} n(x,y)\sqrt{1+y_x^2}dx \,\middle|\, y(x_0)=y_0; y(X)=Y \right\}$$

define surfaces of constant geodesic distance from the point (x_0, y_0).

2. In particular, with the interpretation of Fermat's principle, $S(X,Y)$ is the time required for a *light ray* to travel from (x_0, y_0) to (X, Y); then the level sets define *wave fronts*: set of points that can be reached in the same time. This interpretation is the dual picture of light propagation as introduced by Huygens:

Fermat's principle (1662) : *light rays* ⇔ *extremals of Lagrangian*
Huygens' principle (1690) : *wave fronts* ⇔ *levelsets of value function*

3. Take $(x_0, y_0) = (0, 0)$ for simplicity. In the particular case of a homogeneous medium, with $n(x, y) = n_0$ constant, the light rays are straight lines and S is easily found to be

$$S(X,Y) = n_0\sqrt{X^2+Y^2}.$$

Hence, the wave fronts are circles; $\nabla S(X,Y)$ is normal to the wave front, and satisfies

$$|\nabla S|^2 = n_0^2;$$

the light rays intersect the wave fronts normally.

In the following we will investigate the equation satisfied by the value function. First we derive the result without using the Hamiltonian formulation, then the simpler expressions by using the Hamiltonian.

Total variation of a Lagrangian functional

The family of extremals defines a velocity field in each point:

$$V(T,Q) := \dot{q}(T), \text{ with } q \text{ the extremal through } (T,Q).$$

Along one extremal the total change of S is easily found in lowest order to be

$$dS(T,Q) \equiv S(T+dT, Q+dQ) - S(T,Q) = L(Q, V(T,Q))dT$$

where dS is the change between successive points (T, Q) and $(T + dT, Q + dQ)$, where (in order that both points ly on the same extremal)

$$dQ = V(T,Q)dT.$$

Variations of S at fixed T, variation dQ, is found from

$$\int_{t_0}^{T}[L(q+\delta q,\dot q+\delta\dot q)-L(q,\dot q)]dt=\int_{t_0}^{T}[L_q(q,\dot q)\delta q+L_v(q,\dot q)\delta\dot q]dt$$

$$\begin{array}{rccc} = & \int_{t_0}^{T}[L_q(q,\dot q)\delta q-\partial_t\{L_v(q,\dot q)\}\delta q]dt & + & L_v(Q,V(T,Q))dQ \\ = & 0 & + & L_v(Q,V(T,Q))dQ \end{array}$$

and so

$$\frac{\partial S}{\partial Q}(T,Q)=L_v(Q,V(T,Q)).$$

Combining the results above with

$$dS(T,Q)=\frac{\partial S}{\partial Q}(T,Q)dQ+\frac{\partial S}{\partial T}(T,Q)dT$$

it follows that

$$\left\{\begin{array}{rcl} \frac{\partial S}{\partial Q}(T,Q) & = & L_v(Q,V(T,Q)) \\ \frac{\partial S}{\partial T}(T,Q) & = & L(T,Q)-\frac{\partial S}{\partial Q}(T,Q)V(T,Q) \end{array}\right.$$

and so

$$dS(T,Q)=L_v(T,Q)dQ-[V(T,Q)L_v(T,Q)-L(T,Q)]dT.$$

This formula describes the change in S for independent variations of the two components of the endpoint.

Hamiltonian expressions

Assuming $L(q,v)$ to be a Legendre function in the velocity variable v, let $H(q,p)$ be the Hamiltonian. A momentum field is related to the velocity field according to

$$P(T,Q)=L_v(Q,V(T,Q)).$$

Using the Hamiltonian, the formula for the total variation derived above can be expressed easily as follows

$$dS(Q,T)=P(T,Q)dQ-H(Q,P(T,Q))dT.$$

Consequently

$$\left\{\begin{array}{rcl} \frac{\partial S}{\partial Q}(T,Q) & = & P(T,Q) \\ \frac{\partial S}{\partial T}(T,Q) & = & -H(Q,P(T,Q)). \end{array}\right.$$

Eliminating P in these expressions, a partial differential equation of the first order for S is found:

$$\frac{\partial S}{\partial T}(T,Q)+H(Q,\frac{\partial S}{\partial Q}(T,Q))=0.$$

This equation is known as the *Hamilton Jacobi equation*.

Exercise 120 1. For $q \in IR^N$, and potential $W = W(q)$, the Lagrangian

$$L(q, v) = \frac{1}{2}v^2 - W(q)$$

leads tot the Hamilton Jacobi equation

$$\partial_t S + \frac{1}{2}|\partial_q S(q)|^2 + W(q) = 0.$$

2. Take the special case $W(q) = \frac{1}{2}q^2$ (harmonic oscillator), and $(t_0, q_0) = (0, 0)$. Solve the Euler-Lagrange equation and find directly (for $T < \pi$)

$$S(T, Q) = Q^2 \ cotanT.$$

Interpret this result, in particular the singular behaviour at $T = \pi$.

Exercise 121 Consider once again the geodesic problem in the plane:

$$S(X, Y) = Crit \ \left\{ \int_{x_0}^{X} n(x, y)\sqrt{1 + y_x^2}dx \right| y(x_0) = y_0; y(X) = Y\}$$

defining surfaces of constant geodesic distance from the point (x_0, y_0).

1. Show that the Hamiltonian and momentum are given by

$$H = -\sqrt{n^2 - p^2}, \quad p = y_x H.$$

2. The normal to a level set of S is proportional to

$$\nabla S = (S_X, S_Y) = (-H, P),$$

while the tangent to an extremal $(x, Y(x))$ is $(1, Y_x)$. Conclude from this that *the extremals are perpendicular to the wave fronts*, i.e. perpendicular to the level sets of S.

3. Show that the Hamilton-Jacobi equation reads

$$|\nabla S(x, y)|^2 = n^2(x, y).$$

the so-called *eiconal equation.*

4. Verify that the results are in agreement with those found for a homogeneous medium, with $n(x, y) = n_0$ constant.

5. *Chain line.*
   Consider a chain of given length, fixed at one end point in the origin, the other end point at a position (to be found) on a given circle. Determine from the principle of minimal potential energy the boundary condition for the end point at the circle.

Exercise 122 An alternative derivation of the formulas above is found by using directly the canonical action principle as follows.

1. Observe that the value function S is also defined by

$$S(T,Q) = Crit\ \left\{ \int_{t_0}^{T} [p\dot{q} - H(q,p)]dt \middle| \, q(t_0) = q_0, q(T) = Q; p \right\}$$

2. The integrand can be seen as a line integral of a vector-field along a trajectory $(t, q(t))$:

$$pdq - H(q,p)dt = (-H, p) \cdot (dt, dq).$$

   Show that one of Hamiltons equations, viz.

$$\dot{p} = -\frac{\partial H}{\partial q}(q,p),$$

   is the condition in order that the vector field $(-H, p)$ is conservative.

3. Hence, when for given trajectory $(t, q(t))$ the function $p(t)$ satisfies this equation, the integral is independent of the trajectory and depends only on the end points; this is called Hilbert's independent integral.

4. Then show that, in the notation above,

$$dS(T,Q) = PdQ - H(Q,P)dT,$$

   from which it follows that S satisfies the Hamilton Jacobi equation.

7.5 Exercises

1. *Integrated Euler-Lagrange equation in terms of canonical variables* Suppose that the Lagrangian $L = L(q,v)$ has Legendre transform $H(q,p)$ as above. Referring to Exercise 1 of Chapter 2, show that from the canonical action principle, critical points with respect to p leads to

$$\dot{q} = \frac{\partial H}{\partial p},$$

while for critical points with respect to q, using the Lemma of DuBois-Reymond, it follows that

$$p(t) = -\int^t \frac{\partial H}{\partial q} d\tau + \text{ } constant,$$

the integrated version of the other Hamilton equation.
Hence it follows that the momentum is continuous (even if q is only known to be piecewise differentiable). This is known as *first Weierstrasz-Erdmann Eck-condition.* Show that then actually q and p are differentiable, and q even twice differentiable.

2. *Obstacle problem*
Reconsider the obstacle problem Ex.104 by investigating the value function

$$S(X,Y) = \inf \left\{ \int_0^X u_x^2 dx \middle| u(0) = 0; u(X) = Y \right\},$$

and considering its restriction to the graph of the obstacle ψ:

$$x \mapsto S(x, \psi(x)).$$

Investigate how the free boundary point a can be found in this way.

3. *Dual variational principle*
Consider for given Legendre function F with dual F^*, and $\lambda \neq 0$ the functional

$$\mathcal{J}(u) = \int_0^1 [F(u_x) - \frac{1}{2}\lambda u^2] dx, \quad for \ \ u \in C_0^1([0,1]).$$

   (a) A critical point of $\mathcal{J}$ satisfies

$$\begin{cases} -\partial_x f(u_x) & = & \lambda u, \\ u(0) = u(1) & = & 0 \end{cases}$$

   where $f = F'$.

   (b) Introduce $v \equiv f(u_x)$, and show that v satisfies the equation

$$-\partial_x^2 v = \lambda (F^*)'(v).$$

   Determine the correct boundary conditions for v.

   (c) Note that the boundary value problem for v characterizes the critical points of the functional

$$\hat{\mathcal{J}}(v) = \int_0^1 [\frac{1}{2} v_x^2 - \lambda F^*(v)] dx$$

   on a suitable space of functions v.

(d) Show that the same result can be obtained by performing the Legendre transformation in the functional itself (interchange the order of taking the variations with respect to u and v in the functional in the middle):

$$\begin{aligned} \mathrm{Crit}_u \mathcal{J}(u) &= \mathrm{Crit}_{u,v} \int_0^1 [u_x v - F^*(v) - \tfrac{1}{2}\lambda u^2]dx \\ &= \mathrm{Crit}_v \int_0^1 [\tfrac{1}{2}\tfrac{1}{\lambda}v_x^2 - F^*(v)]dx. \end{aligned}$$

(e) Give the detailed formulae for the special case $F(t) = \frac{1}{2}t^2$, and $F(t) = \frac{1}{4}t^4$.

The above can be generalized as follows.
For given Legendre functions F and G, consider

$$\mathcal{J}(u) = \int [F(u_x) - G(u)], \quad u(0) = u(1) = 0,$$

$$\hat{\mathcal{J}}(v) = \int [G^*(-v_x) - F^*(v)].$$

Show that the critical points u of $\mathcal{J}$ and the critical points v of $\hat{\mathcal{J}}$ are in a one-to-one correspondence, given by

$$v = F'(u_x), \quad u = (G^*)'(-v_x).$$

Show this by using the corresponding boundary value problems, and, alternatively, by a direct investigation of the functionals.

4. *Dual formulation of constrained problems*
Consider the value function of the constrained minimization problem

$$h(\gamma) = \inf \ \{H(u) | \ I(u) = \gamma\}.$$

(a) Verify the following steps that leads to a specific expression for its dual function:

$$\begin{aligned} h^*(\lambda) &= \sup_\gamma[\gamma\lambda - h(\gamma)] = \sup_\gamma \sup_{u,I(u)=\gamma}[\lambda\gamma - H(u)] \\ &= \sup_u[\lambda I(u) - H(u)] \end{aligned}$$

and hence

$$h^*(\lambda) = -\inf_u[H(u) - \lambda I(u)].$$

(b) Observe that if h is convex, then the constrained critical point is also an unconstrained critical point of $H - \lambda I$ for

$$\lambda = h'(\gamma).$$

(c) Compare the results with those obtained in Section 2.4. .

5. *Kinetic energy for free surface flow*
   Consider in the plane a box with free upper boundary described as the graph of a function η:

   $$\Omega(\eta) = \{\ (x,y)\ \mid\ a \le x \le b,\ 0 \le y \le \eta(x)\ \}.$$

   Incompressible, irrotational flow in this box can be described with a flow potential Φ, (velocity $= \nabla\Phi$), satisfying

   $$\Delta\Phi = 0 \quad in \quad \Omega,$$

   and homogeneous Neumann boundary conditions at the vertical boundary and the bottom.
   Let $\phi(x) \equiv \Phi(x, \eta(x))$ be the potential at the free surface. Giving ϕ and η determines the flow, and hence the total kinetic energy.

   (a) Show that the kinetic energy is given by

   $$K(\phi,\eta) = \inf \left\{ \int_{\Omega(\eta)} \frac{1}{2} |\nabla\Phi|^2 \,\middle|\, \Phi(x,\eta(x)) = \phi(x) \right\}$$

   (b) Calculate the variational derivative with respect to ϕ (keeping η fixed).

   (c) Calculate the variational derivative with respect to η (keeping ϕ fixed).
   HINT: First calculate the "total variation" of the functional, and use the result above.

6. *Higher order Lagrangian systems*
   Let L be a given, smooth function of 3 (sets) of variables (position, velocity, acceleration)

   $$(q, v, a) \mapsto L(q, v, a),$$

   and consider the dynamical system (higher order Lagrangian system) for which the evolution equations follow from the action principle

   $$\mathrm{Crit}_q \int L(q, \dot{q}, \ddot{q}) dt.$$

   (Neglect boundary conditions for simplicity).

   (a) Specialize the answers to the following questions for the case

   $$L(q, v, a) = \frac{1}{2} a^2 + F(q, v),$$

   where F is a given, arbitrary function.

(b) Derive the governing 4-th order differential equation for q.

(c) The aim is to derive a Hamiltonian formulation for the system, i.e. to find canonical variables (q_1, q_2, p_1, p_2) and a Hamiltonian $H(q_1, q_2, p_1, p_2)$ such that Hamiltons equations are equivalent to the 4-th order evolution equation for q.
To that end, suppose that L is a Legendre function with respect to the variable a, and define the dual function (Legendre transform)

$$\begin{aligned} L^*(q,v,\alpha) &= \sup_a [\alpha a - L(q,v,a)] \\ &= \alpha a - L(q,v,a) \;\; \textit{for} \;\; \alpha = L_a(q,v,a). \end{aligned}$$

Observe that the action principle can be rewritten like

$$\mathrm{Crit}_q \int L(q,\dot q,\ddot q)dt = \mathrm{Crit}_{(q,p_2)} \int [\ddot q p_2 - L^*(q,v,p_2)]dt$$

$$= \mathrm{Crit}_{(q_1,q_2,p_1,p_2)} \int [\dot q_2 p_2 + p_1(\dot q_1 - q_2) - L^*(q_1,q_2,p_2)]dt.$$

(d) Define the Hamiltonian as suggested by the result above, and verify the governing equations.

(e) The original problem can actually also be interpreted as a constrained Lagranian system: for $q_1 \equiv q, q_2 \equiv \dot q$:

$$L = L(q_1, q_2, \dot q_2), \;\; \textit{with} \;\; q_2 = \dot q_1.$$

Relate this observation to the above result.

(f) Could you have obtained the same result by looking at the original 4-th order equation like

$$\frac{\partial L}{\partial q} - \frac{d}{dt}[\ldots] = 0$$

etc.?

(g) In an anologous way one can find Hamiltonian formulations for Lagrangians L depending on higher order derivatives.

Chapter 8

Functional analytic aspects

In this chapter we make some of the theory of the foregoing chapters more rigorous by using functional analytic tools. After a summary of the main notions and results of (linear) functional analysis, we consider the existence problem, by generalizing Weierstrasz theorem. Then we reconsider the notion of first derivative and variational derivative in light of Riesz' representation theorem in Hilbert spaces.

8.1 Summary Banach and Hilbert spaces

Recall the following definitions and facts.

Definition 123 *Let $\mathcal{U}$ be a linear space. A* norm *on $\mathcal{U}$ is a mapping $|| \ || : \mathcal{U} \to IR$ that has the following properties:*

$$
\begin{aligned}
&||u|| \geq 0, \quad ||u|| = 0 \Leftrightarrow u = 0,\\
&||\lambda u|| = |\lambda| ||u||, \quad \text{for} \quad \lambda \in IR,\\
&||u + v|| \leq ||u|| + ||v||
\end{aligned}
$$

A Banach space *$\mathcal{B}$ is a normed linear space that is complete: Cauchy sequences converge to a limit in $\mathcal{B}$.*

Having a norm available, continuity (of functionals, and of mappings between Banach spaces) can be defined in an obvious way.

Definition 124 *The* algebraic dual *of a Banch space $\mathcal{B}$ is the set of all linear functionals.*
The topological dual *is the completed Banach space $\mathcal{B}^*$ of linear functionals, endowed with the norm*

$$||\ell||_{\mathcal{B}^*} = \sup_{u \in \mathcal{B}} \frac{\ell(u)}{||u||}.$$

The topological dual will be denoted by $\mathcal{B}^*$*; the action of a functional is usually denoted by*

$$\ell(u) \equiv \langle \ell, u \rangle.$$

The Banach space $\mathcal{B}$ *is called a* reflexive Banach space *if the bidual is the space itself:* $\mathcal{B}^{**} \equiv \mathcal{B}$.

Except from convergence in norm, the notion of weak convergence is of extreme importance. We will only need the weak convergence of sequences.

Definition 125 *A sequence* $\{u_n\}_n$ *in* $\mathcal{B}$ *is said to converge weakly to a limit* $\hat{u} \in \mathcal{B}$ *if for all* $\ell \in \mathcal{B}^*$, $\langle \ell, u_n \rangle \mapsto \langle \ell, \hat{u} \rangle$ *for* $n \mapsto \infty$.

Proposition 126 *Any strongly convergent sequence converges weakly; the converse is only true in finite dimensional spaces. Weak limits of sequences are unique.*

As is known, a bounded sequence in an infinite dimensional space does not need to have a subsequence that converges in norm. However, there is a subsequence that converges weakly in a reflexive Banach space; this property characterizes such spaces.

Proposition 127 *A Banach space is reflexive iff the unit ball is weakly compact (i.e. compact with respect to the weak topology (of sequences)).*

Definition 128 *An* inner product *on the space* $\mathcal{U}$ *is a bilinear, symmetric mapping* $(\ ,\ ) : \mathcal{U} \times \mathcal{U} \to \mathcal{R}$ *that is positive:* $(u, u) > 0$ *for* $u \neq 0$.
A Hilbert space *is an inner product space that is complete with respect to the inner product norm.*

The norm is w.l.s.c. (but not weakly continuous).

Proposition 129 *A Hilbert space is a reflexive Banach space: the unit ball is weakly compact.*

Theorem 130 Riesz
The dual of a Hilbert space $H, (\ ,\ )_H$ *can be identified with* H*: for every continuous linear functional* $\ell \in H^*$ *there exists an element* $u_\ell \in H$ *such that*

$$\ell(v) = (u_\ell, v)_H \quad \textit{for all} \quad v \in H.$$

Exercise 131 *1.* The space $C^m(I)$ of m-times continuously differentiable functions on an interval I is a Banach space with norm

$$|u|_{C^m} = \sum_{k=0}^{m} |\partial_x^k u|_\infty,$$

where the sup norm $|\ |_\infty$ is given by

$$|u|_\infty = \sup_{x \in I} |u(x)|.$$

This norm cannot be derived from an inner product (prove!).

2. $L_2(\Omega)$ is the Hilbertspace of functions on Ω, endowed with the ususal innerproduct and norm:

$$\langle u,v\rangle \equiv (u,v)_{L_2} = \int_\Omega u(x)v(x)dx$$

3. Functions from L_2 are not necessarily continuous; hence the restriction of a function to a specific point is not a continuous functional! Give examples.

8.2 Generalizations of Weierstrasz' theorem

We recall the definition of a minimizer of a functional on a subset of some linear space.

Definition 132 *Let $\mathcal{M}$ be a non-empty subset of some linear space $\mathcal{U}$, and F a (real-valued) function(al) defined on $\mathcal{U}$ (or $\mathcal{M}$). We say that there exists a solution $\hat{u} \in \mathcal{M}$ of the minimization problem for F on $\mathcal{M}$ if the infimum*

$$\mu := \inf \ \{ \ F(u) \ \mid \ u \in \mathcal{M} \ \} \tag{8.1}$$

is finite and attained for $\hat{u}$:

$$\mu = F(\hat{u}) \leq F(u) \ \ \textit{for all} \ \ u \in \mathcal{M}. \tag{8.2}$$

Notation: $\hat{u} \in$Min $\{ \ F(u) \ \mid \ u \in \mathcal{M} \ \}$.

In the next result we generalize the result of Weierstrasz that in a finite dimensional space a continuous function attains its maximum and its minimum on any compact (bounded and closed) set. The generalization is in various directions: continuity is replaced by semi-lower continuity, compactness by weak compactness and unbounded domains can be dealt with if the functional is coercive.

Proposition 133 Generalizations of Weierstrasz' theorem
*If one of the conditions **C-*** on F and $\mathcal{M}$ that are listed below is satisfied, there exists at least one solution of the minimization problem (8.1).*

To appreciate the conditions to follow, we first sketch the general structure of the proof.
Idea of proof:
Let $\{u_n\}$ be a *minimizing sequence*, i.e. $u_n \in \mathcal{M}$ and $F(u_n) \mapsto \mu$. The conditions will guarantee that (i) there exists a subsequence $\{u_{n'}\}$ that is convergent in $\mathcal{M}$ (in some topology), say to an element $\hat{u}$, and that then (ii) $F(\hat{u}) \leq \liminf F(u_{n'})$.

Conditions:

1. **C-1:** $\mathcal{M}$ is a finite set, no conditions on F.
2. **C-2:** $\mathcal{M}$ is a compact subset of $\mathcal{R}^n$ and F is continuous.

3. **C-3:** $\mathcal{B}$ is a Banach space, $\mathcal{M}$ is a compact subset of $\mathcal{B}$ and F is lower semi-continuous (l.s.c.).
4. **C-4:** $\mathcal{B}$ is a reflexive Banach space, $\mathcal{M}$ is a weakly closed subset of $\mathcal{B}$, F is lower semi-continuous with respect to weak convergence (w.l.s.c.), and F is coercive on $\mathcal{M}$:

$$F(u) \mapsto \infty \text{ for } u \in \mathcal{M}, \; |u| \mapsto \infty \tag{8.3}$$

5. **C-5:** $\mathcal{B}$ is a Banach space, $\mathcal{M}$ a bounded, closed, *convex* set, F is l.s.c. and *convex.*

Exercise 134 *1.* Prove the result for the Conditions C-1 up to C-4.

2. For C-5, use the following

Lemma 135 Mazur
A convex combination of the elements of a weakly convergent sequence converges in norm to the weak limit.

and the following consequence:

Proposition 136 *A functional that is l.s.c. and* convex *is w.l.s.c..*

8.2.1 Quadratic functionals and forms

Let H be a Hilbert space, dual H^*. As a consequence of Riesz' theorem, it holds that for a continuous, bilinear functional $b : H \times H \mapsto IR$ there exists a unique bounded (continuous) linear map $A : H \mapsto H^*$ such that

$$b(u, v) = \langle Au, v\rangle. \tag{8.4}$$

If, moreover b is symmetric, A is self-adjoint. In that case

$$a : H \mapsto IR, \quad a(u) := b(u, u) = \langle Au, u\rangle \tag{8.5}$$

is called a *quadratic form.*

Proposition 137 *Let a be a continuous quadratic form that is* strictly positive *in the sense that for some $c > 0$ $a(u) \geq c||u||_H^2$ for all $u \in H$, A is called H-elliptic in that case. Then for any $\ell \in H^*$ the quadratic functional $u \mapsto a(u) - \ell(u)$ is bounded from below on H and there exists a unique minimizer: the unconstrained minimization problem*

$$Min \; \{a(u) - \ell(u) | u \in H\}$$

has a solution.

Exercise 138 *1.* First prove the following.

> ***Lemma 139*** *If a is a quadratic continuous form that is* non-negative*, this quadratic form is weakly l.s.c..*

2. Prove the proposition.

3. Prove the existence of a minimizer of *Dirichlet's problem:*

$$Min \left\{ \int_\Omega [\frac{1}{2}\sigma|\nabla u|^2 - \rho(x)u]dx \right| u(x) = 0, \ \ for \ \ x \in \partial\Omega\}$$

when σ is strictly positive on Ω, and ρ continuous.

8.2.2 Sobolew spaces and Rellich's embedding

For simplicity we restrict to functions of only one variable.

The *Sobolew space* $H^1([0,1], [H^1_0([0,1])]$ is the Hilbert space with innerproduct

$$(u,v)_{H^1} = \int_0^1 [u_x(x)v_x(x) + u(x)v(x)]dx,$$

and is obtained as the completion of the continuous differentiable functions u [with $u(0) = u(1) = 0$] under the innerproduct norm.
(On $H^1_0([0,1]$ an equivalent norm is $\langle u, v\rangle = \int_0^1 u_x(x)v_x(x)dx$.)

With elementary estimates one can prove the following results.

Proposition 140 Poincaré (-Friedrichs-Wirtinger) inequalities
For functions $u \in C^1([0,1])$ *the following inequalities hold for suitable constants* c_1, c_2, c_3*:*

$$|u|^2_\infty \leq c_1 \int u_x^2$$

$$\int u^2 \leq c_2 \int u_x^2$$

$$|u|^2_\infty \leq c_3 \int u_x^2$$

Exercise 141 Prove the inequalities.Note that the problem to find the "best" constants in the inequalities above is a variational problem itself.

In the completion process from C^1 to H^1 these inequalities remain true, showing the result that $H^1_{[0]}([0,1])$ is *continuously* embedded in $C^0_{[0]}([0,1])$. The following stronger statement holds (for functions of *one* (!) scalar variable).

Lemma 142 Rellich
$H^1_{[0]}([0,1])$ *is* compactly *embedded in* $C^0_{[0]}([0,1])$*: sequences bounded in* $H^1_{[0]}([0,1])$ *have subsequence that converges in* $C^0_{[0]}([0,1])$.

A direct consequence is the following.

Proposition 143 *For any continuous function* f*, the functional* $\int_0^1 f(u(x),x)dx$ *defined on* H^1 *is continuous w.r.t. weak convergence, i.e. weakly continuous.*

Exercise 144 Prove this Proposition, and use it extensively in the following applications.

1. The minimization problem

$$\inf \ \left\{\int [\frac{1}{2}u_x^2 - f(u)]dx \right| u(0) = u(1) = 0\}$$

has a solution if f is bounded from above or if f is sub-quadratic at infinity:

$$\frac{f(u)}{u^2} \mapsto 0 \ \ for \ \ |u| \mapsto \infty.$$

In particular, there exists a solution if f is linear in u, i.e. if $f(u,x) = g(x)u$ for any smooth function g on $[0,1]$.
(Note that for any function f the *supremum* of this functional is infinite: the maximization problem is not well defined.)

2. For each function f the constrained minimization problem

$$\inf \ \int \frac{1}{2}u_x^2 \int f(u) = \gamma, u(0) = u(1) = 0\Big\}$$

has a solution for all $\gamma \in$ the interior of the range of f.

3. *Euler buckling.* .
The constrained minimum

$$\inf\{\int \frac{1}{2}u_x^2 \int [1-\cos(u)] = \gamma, u(0) = u(1) = 0\Big\}$$

exists and is non-trival for each $0 < \gamma < 2$.
The unconstrained minimizer of

$$\inf\{\int [\frac{1}{2}u_x^2 - \lambda f(u)]dx \ u(0) = u(1) = 0\}$$

exists for all λ but is only non-trivial if $\lambda > \lambda_1 := \pi^2$.

4. *KdV cnoidal waves*
Prove the existence of a solution of the problem for periodic travelling wave shapes for the KdV-equation*:*

$$Mi\int_0^1 [\frac{1}{2}u_x^2 - u^3] \int u = 0, \ \int \frac{1}{2}u^2 = \gamma, \ u(0) = u(1).\Big\}$$

8.3 Differentiability, criticality conditions

8.3.1 Gateau and Frechet differentiability

Let N be a map from a linear space X into Y. The *formal derivative* of N at $x \in X$ in the direction $\eta \in X$ is defined as (and denoted by)

$$DN(x)\eta := \frac{d}{d\varepsilon} N(x + \varepsilon\eta)\bigg|_{\varepsilon=0}$$

whenever this derivative exists.
When $DN(x)$ is a linear, continuous map from X into Y, it is called the *Gateaux drivative*;
when DN as a map from X into $L(X, Y)$ is continuous at x, it is the usual *Frechet derivative.*

8.3.2 Gradient of functionals

Specialized to functionals F, i.e. $Y = \mathcal{R}$, (nomenclature and notation motivated by the classical Calculus of Variations, dealing with density functionals):
the *first variation*

$$\delta F(u; \eta) = \frac{d}{d\varepsilon} F(x + \varepsilon\eta)\bigg|_{\varepsilon=0} \tag{8.6}$$

and the *second variation*:

$$\delta^2 F(u; \eta) = \frac{d^2}{d\varepsilon^2} F(x + \varepsilon\eta)\bigg|_{\varepsilon=0}. \tag{8.7}$$

In a Hilbert space, the first variation defines the gradient of a functional by using Riesz' theorem; this notion depends on the inner product that is used. In particular it must be distinguished from the variational derivative for density functionals (for which, apart form boundary contributions, the L_2-inner product is used).

Proposition 145 *Let $X = H$ be a Hilbert space, and suppose that the first variation $\eta \mapsto \delta F(u; \eta)$ is linear and continuous (i.e. Gateaux differentiable). Then there exists an element, called the* gradient *of F at u, grad $F(u)$, such that*

$$\delta F(u; \eta) = (\mathit{grad}\ F(u), \eta)_H.$$

When Frechet differentiable, grad F is a continuous *map in H.*

Exercise 146 *1.* In a Hilbert space, with norm $||\ ||_H$ it holds for all $u \in H$ that

$$\mathit{grad}\ ||u||^2 = 2u.$$

2. In particular, for $H^1([0,1])$

$$\textit{grad} \int \frac{1}{2}(u_x^2 + u^2)dx = u.$$

3. For functions u with $u(0) = u(1) = 0$, and differentiable function f we have

$$\textit{grad} \int f(u)dx = \zeta(u), \quad \textit{with } \zeta \ \textit{ the solution of } \ (-\partial_x^2 + 1)\zeta = f'(u).$$

8.3.3 Variational derivative

Let $H \subset V$, with H and V both Hilbert spaces. We identify V^* with V (Riesz), and use the inner product of V (denoted by $\langle \ , \ \rangle$) to reformulate the gradient. Then V is said to be the *pivot space*.
Since then $H^* \supset V$, so in total

$$H \subset V = V^* \subset H^*, \tag{8.8}$$

there is an element $\delta F(x) \in H^*$, called the *variational derivative* of F at x satisfying

$$\delta F(x;\eta) = \langle \delta F(x), \eta \rangle \quad \text{for all } \ \eta \in H.$$

When dealing with function spaces (functions defined on a domain $\Omega \subset \mathcal{R}^n$, say) and density functionals, it is natural to take for V the function space with the $L_2(\Omega)$- inner product. This is what we have done in the previous chapters, and also in the following the phrase ariational derivative will be restricted to this case. (It is also used in less well defined situations, and δF is in most cases a distribution.)
As seen before, to prevent boundary contributions when performing partial integrations, the defining expression for δF is restricted to functions $\eta \in C_0^\infty(\Omega)$, where $C_0^\infty(\Omega)$ is the set of *test functions* on the domain Ω: functions infinitely differentiable with compact support in Ω. Hence, as before,

$$\delta F(u;\eta) = \int_\Omega \delta F(u)(x)\eta(x)dx, \quad \text{for all } \ \eta \in C_0^\infty(\Omega).$$

Exercise 147 *1.* The dual of $H_0^1([0,1])$ is $(H_0^1)^* = H^{-1}$, a space of distributions; with that meaning:

$$\delta \int [\frac{1}{2}u_x^2 + u^2]dx = -u_{xx} + u$$

and

$$\delta \int [\frac{1}{2}u_x^2 - f(u)]dx = -u_{xx} - f'(u).$$

Observe the difference with the gradient of these functionals whn the H^1-inner product is used.

2. For the point-evaluation $F(u) = u(a), a \in (0,1), u \in H^1([0,1])$,

$$\delta F(u)(x) = \delta_{Dirac}(x-a).$$

8.3.4 Unconstrained critical points

We briefly recall and rephrase some previous results.

Definition 148 *A point $\hat{x}$ is called a critical point of F on linear space X if*

$$\delta F(\hat{x},\eta) = 0 forall \eta \in X.$$

In a Hilbert space this is equivalent to

$$grad\ F(\hat{x}) = 0,$$

while in a functions space "necessarily" (up to natural boundary conditions) $\delta F(\hat{x}) = 0$.

Remark 149 For density functionals, $\delta F(\hat{x}) = 0$ follows from $\delta F(\hat{x},\eta) = 0$ for all $\eta \in X$ provided $\delta F(\hat{x})$ is a continuous function, and provided X contains all test functions, as a consequence of the Lagrange's Lemma, as we have seen.

8.3.5 Constrained critical points

We now consider constrained extremal problems. Different from the previous chapters, we now allow sets that are not necessarily intersections of level sets of functionals. The following formulation is much more general.

Let $N : X \mapsto Y$, and $\mathcal{M} := \{x \in X \mid N(x) = y_0\}$ be non-empty. A point $\hat{x} \in \mathcal{M}$ is called a *regular point* if N is Frechet differentiable at $\hat{x}$ with a derivative $DN(\hat{x}) : X \mapsto Y$ that has closed range in Y. In particular, assume that $DN(\hat{x})$ maps X *onto* Y. Then

$$\ker(DN(\hat{x}))^{\perp} = \text{range } (DN(\hat{x})^*),$$

where $\ker(DN(\hat{x}))^{\perp} \equiv \{\ell \in X^* \mid \ell(\eta) = 0 \quad \text{for all} \ \ \eta \in \ker(DN(\hat{x}))\}$.
In that case, $T_{\hat{x}}\mathcal{M} = \ker(DN(\hat{x}))$ where $T_{\hat{x}}\mathcal{M}$ is the *tangent space* at the point $\hat{x}$ to $\mathcal{M}$ (*Lemma Lyusternik*).

Definition 150 *A point $\hat{x}$ is called a* critical point *of F on the set $\mathcal{M} = \{x \in X \mid N(x) = y_0\}$ if*

$$\delta F(\hat{x},\eta) = 0 \ \ \textit{for all} \ \ \eta \in T_{\hat{x}}\mathcal{M}. \tag{8.9}$$

Proposition 151 *If $\hat{x}$ is a solution of the minimization probem of F on $\mathcal{M}$, then it is a critical point. If $\hat{x}$ is a regular point of $\mathcal{M}$,* Lagrange's multiplier rule *holds*[1]*: there exists a multiplier $\lambda \in Y^*$ such that for all ζ:*

$$\delta F(\hat{x};\zeta) = \langle DN(\hat{x})\zeta, \lambda\rangle. \tag{8.10}$$

Equivalently, in a Hilbert space

$$grad\ F(\hat{x}) = DN(\hat{x})^*\lambda \tag{8.11}$$

while for density functionals:

$$\delta F(\hat{x}) = DN(\hat{x})^*\lambda \tag{8.12}$$

(the adjoint being defined with respect to the L_2-inner product).
For the minimizer the constrained second variation is non-negative on the tangent space:

$$\delta^2[F - \langle N, \lambda\rangle](\hat{x};\eta) \geq 0, \quad \text{for all} \ \ \eta \in T_{\hat{x}}\mathcal{M}. \tag{8.13}$$

The specialization to the case considered in Chapter 2 is as follows.
Let $(K_1, \ldots, K_p) : H \mapsto \mathcal{R}^p$ be a set of differentiable functionals. A point $\hat{x}$ is a regular point of the manifold $\mathcal{M} := \{x \mid K_r(x) = \gamma_r, 1 \leq r \leq p\}$ if the derivatives at $\delta K_r(\hat{x};\cdot) \in H^*$ are linearly independent.

Proposition 152 *For a critical point $\hat{x}$ of F on $\mathcal{M}$ there exists multipliers $(\sigma_1, \ldots, \sigma_p)$ such that*

$$\delta F(\hat{x};\cdot) = \sum_r \sigma_r \delta K_r(\hat{x};\cdot)\mathrm{on}H.$$

Equivalently, in a Hilbert space,

$$grad\ F(\hat{x}) = \sum_r \sigma_r grad\ K_r(\hat{x}),$$

and for density functionals:

$$\delta F(\hat{x}) = \sum_r \sigma_r \delta K_r(\hat{x}).$$

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[1] Just as before, Lagrange's multiplier rule can be seen as a method to determine the equation for a *constrained* critical point: $\mathcal{M} \ni x \mapsto F(x)$ as the equation for an *unconstrained* critical point of a *Lagrangian functional* that is now given for $\lambda \in Y^*$ by

$$X \ni x \mapsto F(x) - \langle N(x), \lambda\rangle.$$

8.4 Periodic Hamiltonian motions

We now give a few, more difficult, examples of optimization problems in dynamics for which the existence of a critical point can be proved. In some way or another, we prove the existence of a periodic motion of a classical Hamiltonian system by using (variants of) the action functional.
Note that the restriction to *periodic* solutions (whether the period is prescribed in advance, or when it is not prescribed but has to found as part of the solution) makes the problem to one with *boundary* conditions, different from the *initial* value problem that is usually considered; for an initial value problem *local existence* on a sufficiently *small* time interval around the initial time can be proved with the ususal contraction argument. But for a boundary value problem, the difficulty in the proof of existence is the fact that existence of a solution on the periodic interval is a problem of existence of a *global solution*.
A second observation is that usually the periodic solution is a saddle point of the action functional, while Weierstrasz theorem can only give results for minimizers (or maximizers). By transforming the problem in various ways, we will be able to reformulate the saddle point as a minimizer on a suitably restricted subset.

In historic perspective, this specific application has lead to many new developments in variational methods over a period of more than two centuries.

We recall briefly the general setting.
The *position* of mass points (all masses normalized to 1 for simplicity) is described by a vector from the *configuration space*: $q \in I\!R^n$. The *state* of the dynamic system is described by a point in the state-, or *phase space*: $(q,p) \in I\!R^n \times I\!R^n$, where p has the meaning of momentum (velocity $\dot{q}$).
For given (smooth) potential energy function $V = V(q,t)$, defined on configuration space and possibly depending on time (forcing), consider solutions of the following *Hamiltonian system*, equivalently formulated on configuration space (as Newton-like equation, 2-nd order in time) and on phase space (Hamilton formulation, 1-st order in time):

$$-\ddot{q} = V'(q,t), \quad \text{resp} \quad \left\{ \begin{array}{lcl} \dot{q} & = & p \\ \dot{p} & = & -V'(q,t) \end{array} \right. \tag{8.14}$$

These systems arise from a dynamic variational principle: the equations are the Euler-Lagrange equations of the *action functional* on configuration space:

$$\mathcal{A}(q) = \int [\frac{1}{2}|\dot{q}|^2 - V(q,t)]dt \tag{8.15}$$

resp the *canonical action functional* on phase space:

$$\mathcal{CA}(q,p) = \int [p \cdot \dot{q} - V(q,t)]dt. \tag{8.16}$$

Periodic solutions

When V depends periodically on time, period T say, it is possible to look for solutions that are T-periodic. (When V is autonomous, T is not given a priori.) Finding T-periodic solutions reduces the problem to a boundary-value problem on the compact interval $t \in [0, T]$, with boundary conditions:

$$\left\{ \begin{array}{lcl} q(0) & = & q(T) \\ \dot{q}(0) & = & \dot{q}(T) \end{array} \right. \quad \textit{resp.} \quad \left\{ \begin{array}{lcl} q(0) & = & q(T) \\ p(0) & = & p(T) \end{array} \right. \tag{8.17}$$

and are obtained as critical points of

$$\text{Crit } \left\{ \mathcal{A}(q) | \; q(0) = q(T) \right\}, \quad \text{resp Crit } \left\{ \mathcal{CA}(q,p) | \; q(0) = q(T) \right\}.$$

Note that the remaining boundary conditions arise as *natural boundary conditions*.

In particular when V is autonomous, special periodic solutions can be considered that are simple continuations of the motion on part of the period:
Brake orbits: motion between restpoints, satisfying

$$\dot{q}(0) = \dot{q}(T/2) = 0, \text{ resp } . \; p(0) = p(T/2) = 0; \tag{8.18}$$

these boundary conditions are obtained as natural boundary conditions by not prescribing any conditions at all.

If, moreover, V is even in q: $V(q) = V(-q)$, *normal mode solutions* are determined by the motion during a quarter period:

$$q(0) = \dot{q}(T/4) = 0, \quad \text{resp} \quad q(0) = p(T/4) = 0, \tag{8.19}$$

obtained by prescribing only $q(0) = 0$ in the variational principle.

Except for normal modes solutions (when $q(0) = 0$ is prescribed), the functional $\int |\dot{q}|^2$ is not equivalent to the H^1-norm (it vanishes for constant vector functions). In those cases it is natural to split H^1 in an orthogonal way:

$$H^1_T([0,T]) \equiv \{q \in H^1_T([0,T]) \mid q(0) = q(T)\} = I\!R^n + Y_T,$$

with

$$Y_T = \left\{ y \in H^1_T([0,1]) | \int y = 0 \right\},$$

so $q = c + y$, with a constant vector $c \in I\!R^n$ and $y \in Y_T$. Then $\int |\dot{q}|^2 = \int |\dot{y}|^2$ is (equivalent to) the norm in Y_T.

8.4.1 Periodic motions with prescibed period

Proposition 153 *If $V(q)$ is even and subquadratic in q there exists a normal mode solution related to the minimizer (when nontrivial) of*

$$Min \left\{ \int_0^{T/4} [\frac{1}{2}|\dot{q}|^2 - V(q)]dt \middle| \quad q(0) = 0 \right\}$$

The proof of the existence is contained in the previous examples and will not be repeated.

Proposition 154 Periodic potential and forcing.
Suppose $q \mapsto V(q)$ is periodic in each component of q. Let f be a T-periodic function with $\int_0^T f(t)dt = 0$. Then the minimization problem

$$Min \left\{ \int_0^{T} [\frac{1}{2}|\dot{q}|^2 - V(q) - f(t)q(t)]dt \middle| \, q(0) = q(T) \right\} \tag{8.20}$$

has a solution which is a T-periodic solution of the forced equation:

$$-\ddot{q} = V'(q) + f(t).$$

Exercise 155 *1.* Prove the proposition. Observe that by writing $q(t) = c + y(t)$

$$\int_0^T [\frac{1}{2}|\dot{q}|^2 - V(q) - f(t)q(t)]dt = \int_0^T [\frac{1}{2}|\dot{y}|^2 - V(c+y) - f(t)y(t)]dt.$$

Then show that a minimizing sequence $q_k = c_k + y_k$, $\{y_k\}$ is bounded (since V is bounded); finally, from the periodicity of V, the elements $\{c_k\}$ can be taken to be bounded.

2. Note that the special case $f \equiv 0$ leads to a solution for any T. Only for certain values of T, however, the minimizer is non-trivial.

3. A specific example for which the minimizers are not trivial, are periodic solutions of the forced pendulum equation:

$$-\ddot{q} = \sin(q) + f(t).$$

As stated in the introduction, typically, periodic solutions correspond to *saddle points* of the (canonical) action functional. As a first example, the following result; in this case the saddle point can be characterized explicitly (analytically), and transformed to a *naturally constrained minimizer*, i.e. the constraint does not contribute to the governing equation for the critical point.

Proposition 156 *Suppose V is strictly convex and subquadratic at infinity. Then there exists a periodic solution corresponding to a saddle point:*

$$Sad \left\{ \int_0^T [\frac{1}{2}|\dot{q}|^2 - V(q)]dt \middle| q(0) = q(T) \right\}$$

$$= Min_{\ y \in Y_T}\ Max_{\ c \in \mathcal{R}^n} \int_0^T [\frac{1}{2}|\dot{y}|^2 - V(c+y)]dt$$

$$= Min \left\{ \int_0^T [\frac{1}{2}|\dot{q}|^2 - V(q)]dt \middle| q \in H^1_T,\ \int_0^T V'(q) = 0 \right\}.$$

Exercise 157 Prove the proposition above; first prove the existence, then investigate the governing equation to show that the constraint $\int_0^T V'(q) = 0$ is a natural constraint: the multiplier in the equation vanishes.

8.4.2 Periodic motions with prescribed energy

In the following V is autonomous. Then the "energy" is conserved (constant in time) for all solutions:

$$\frac{1}{2}|\dot{q}|^2 + V(q) = E, \quad \text{resp . } H(q,p) \equiv \frac{1}{2}|p|^2 + V(q) = E. \tag{8.21}$$

We try to find periodic solutions, with a priori unknown period T, that have a prescribed value of the energy. It is simplest to normalize the time: $\tau = t/T \in [0,1]$.

Proposition 158 Variational principles on phase space
Up to time-scaling, periodic solutions with prescribed energy E are critical points of

$$Crit \left\{ \int_0^1 p \cdot \dot{q} d\tau \middle| H(q,p) = E, q(0) = q(1) \right\} \tag{8.22}$$

and also of

$$Crit \left\{ \int_0^1 p \cdot \dot{q} \middle| \int_0^1 H(q,p)d\tau = E, q(0) = q(1) \right\} \tag{8.23}$$

In the last case, the (constant) multiplier λ arising from the energy constraint is precisely the period T of the motion.

For fixed $q \in IR^n$ such that $V(q) \leq E$, the supremum over p in the above principles is obtained for the vector collinear with $\dot{q}$:

$$\dot{q} = \lambda p, \quad \text{and} \quad |p| = \sqrt{2(E - V(q))}.$$

Hence, solutions of these optimization problems are obtained if solutions can be found of the following variational problems.

Proposition 159 Variational principles on configuration space
Up to time-scaling, periodic solutions with prescribed energy E are critical points of the following Jacobi functional

$$Crit\ \left\{\int_0^1 \sqrt{2(E-V(q))}|\dot{q}|d\tau \right| \ q(0)=q(1)\} \tag{8.24}$$

and also of

$$Crit\ \{\mathcal{J}_E(q)|\ q(0)=q(1)\} \tag{8.25}$$

where J_E is the following modified Jacobi functional

$$\mathcal{J}_E(q)=[\int_0^1 \frac{1}{2}|\dot{q}|^2 d\tau]*[E-\int_0^1 V(q)d\tau] \tag{8.26}$$

The modified Jacobi functional is essentially easier to investigate (with standard Hilbert space techniques) than the original Jacobi functional (in which the factor $\sqrt{2(E-V(q))}$ can vanish at certain times, and hence does not easily define a norm).
As an example of the use of $\mathcal{J}_E$, the following proposition in which we use "polar coordinates": for $q \in \{q \in H^1([0,1]) \mid q(0)=0\}$, $q=\rho\omega$ with $\omega \in S$, S the unit ball: $S=\{q \mid \int |\dot{q}|^2=1\}$.

Proposition 160 *Assume that $V(x) \geq 0, V(0)=0$ and that V is* strictly convex *and* even. *For any $E>0$ there is a periodic solution with energy E; this solution is a* normal mode *and corresponds to a* saddle point *of J_E:*

$$Sad\ \{\mathcal{J}_E(q)|\ \ q(0)=0\} \tag{8.27}$$

The character of the saddle point can be found explicitly, and can be transformed to a (naturally) constrained minimizer as follows:

$$Min\ _{\omega\in S}\ Max\ _{\rho\geq 0}\ \mathcal{J}_E(\rho\omega) \equiv Min\ \ \{\mathcal{J}_E(q)|\ \ q\in N_E\} \tag{8.28}$$

The set N_E is a natural constraint, explicitly given by

$$N_E=\left\{\ q\ \middle|\ \int[V(q)+\frac{1}{2}V'(q)\cdot q]=E\right\}. \tag{8.29}$$

Exercise 161 Prove the proposition above; first existence, then verify that N_E is a natural constraint.

Chapter 9

Variational Calculus with MAPLE

The basic calculational aspects for functions can be generalized for functionals (functions on infinite dimensional spaces, mostly function spaces).
In this mws we deal with the **first variation** (directional derivative) and the **variational derivative** (the "gradient" of a functional), mainly of socalled density functionals: integrals over a certain interval of expressions of functions defined on that interval.
In this mws. Maple is used to illustrate the algebraic manipulations of the basic calculational aspects.

9.1 First variation

9.1.1 Definition and procedure 'fvar'

For a given functional F, the first variation is nothing but the directional derivative:
The *first variation* of the functional F at a point u in the direction v is denoted by $\delta F(u, v)$ and is the expression (when defined)

$$\delta F(u, v) := \frac{d}{d\varepsilon} F(u + \varepsilon v)\bigg|_{\varepsilon=0} .$$

In Maple-notation we write "fvar(F,u,v)" for $\delta F(u, v)$.

Note that $\varepsilon \to u + \varepsilon\, v$ should be viewed as a line through u in the direction v in the function space. In Maple we have to describe this line as a *parameterized function*:

$$line := \varepsilon \to unapply(u(t) + \varepsilon\, v(t),\, t)$$

and the functional evaluated on this line

$$F(t \to u(t) + \varepsilon\, v(t))$$

has to be differentiated with respect to ε.
In one procedure,with some precautions for general use:

Procedure fvar

```
fvar := proc (F, u, v)
local fv, ε;
fv := unapply(simplify(subs(ε = 0,
diff(F(unapply(U(τ) + εV(τ), τ)), ε))), U, V) ;
fv(u, v)
end;
```

This leads to the result that we want.

Exercise 162 *1.* L2-norm of functions: $L := u \to \int_0^1 u(x)^2\, dx$

$$fvar(L, u, v) = 2 \int_0^1 v(x)\, u(x)\, dx$$

2. Second order derivative, non-quadratic integrand :
$G := u \to \int \left[(\partial_x^2 u(x))^2 + u(x)^4\right] dx$

$$fvar(G, u, v) = 2 \int (\frac{\partial^2}{\partial x^2}\, u(x))\, (\frac{\partial^2}{\partial x^2}\, v(x)) + 2\, u(x)^3\, v(x)\, dx$$

3. Examples from Classical Mechanics

(a) $L := q \to \int \left[\frac{1}{2}\ \dot{q}(t)^2 - \frac{1}{2}\, q(t)^2 - q(t)^3\right]\ dt$

$$fvar(L, q, v) = \int \left[\dot{q}(t)\dot{v}(t) - q(t)\, v(t) - 3\, q(t)^2\, v(t)\right]\ dt$$

(b) $L := q \to \int \left[\frac{1}{2}\, \dot{q}^2 - U(q(t))\right]\ dt$

(c) $L := q \to \int Lag(q(t), \dot{q}(t))\, dt$

$$fvar(L, q, v) = \int\ [D_1(Lag)(q,\ \dot{q})\, v(t) + D_2(Lag)(q, \dot{q})\dot{v}(t)]\ dt$$

9.1.2 Derivative of a functional along a vectorfield (Lie-derivative)

Assuming the function $u(x)$ to depend on an additional parameter (in many applications, t = 'time'), substituting in a functional F reduces the value to a function of t: $F(u(x,\, t)) = f(t)$.

The derivative of f with respect to t is related to the first variation of the functional:

$$\frac{d}{dt}f(t) = \frac{d}{dt}F(u(x,\, t)) = \delta F(u, \partial_t u)$$

This can be seen as a special case of the *chainrule for functionals*.
If the evolution $t \mapsto u(t)$ satisfies a first order equation

$$\frac{\partial}{\partial t}\,u(x,\, t) - K(u(x,\, t)) = 0$$

with vector field K, the time derivative of the functional is known as the "**Lie-derivative**": the *directional derivative along the vectorfield*:

$$\frac{d}{dt}F(u(x,\, t)) = \delta F(u, \partial_t u) = \delta F(u, K(u)).$$

Exercise 163 The restriction of the functional F

$$F := v \rightarrow \int v(x)^3\, dx$$

to an evolution $u := t \rightarrow \mathit{unapply}(w(x,\, t),\, x)$ is given by

$$F(u(t)) = \int w(x,\, t)^3\, dx$$

and a direct differentiation with respect to t provides (the chainrule!!)

$$\partial_t F(u(t)) = \int 3\, w(x,\, t)^2\, (\partial_t w(x,\, t))\, dx$$

For an evolution equation given by:

$$Eq := \partial_t\, w(x,\, t) - K(w(x,\, t)) = 0$$

the result is

$$\partial_t F(u(t)) = \int 3\, w(x,\, t)^2\, K(w(x,\, t))\, dx$$

This is the same as a direct calculation of the Lie-derivative of F along vector field K:

$$\mathit{fvar}(F, u(t), \mathit{unapply}(K(w(x,t)), x)) = 3 \int w(x,\, t)^2\, K(w(x,\, t))\, dx$$

9.1.3 Frechet derivative: linearization procedure for equations (instead of functionals)

The directional derivative defined above for functionals applies just as well to operators, leading to the concept of *formal Frechet derivative.*
This derivative is of extreme importance in the analysis of complicated (sets of) equations that appear in many applications, symbolically: $\mathcal{E}(u) = 0$. The Frechet derivative leads to the *linearized equations*:

$$D\mathcal{E}(u)(v) = 0$$

which is the equation for perturbations v such that $u + \varepsilon\, v$ is in lowest order of ε also a solution of the equation:

$$\mathcal{E}(u + \varepsilon\, v) = \mathcal{E}(u) + \varepsilon\, D\mathcal{E}(u)(v) + \mathcal{O}(\varepsilon^2)$$

Functions of one variable

Procedure lin

```
lin := proc(F, u, v, x) local eps, line, dv;
line := eps- > unapply(U(x) + eps * V(x), x);
dv := unapply(simplify(subs(eps = 0,
diff(F(line(eps))(x), eps))), (U, V, x));
dv(u, v, x);
end;
```

Exercise 164 1. $F(u)(x) := u(x)^2 + u(x)$

$$lin(F, U, \eta, x) = 2\,U(x)\,\eta(x) + \eta(x)$$

2. $F(u)(x) := u(x)^2 + sin(u(x)) + \partial_x\, u(x)$

$$lin(F, U, \eta, x) = 2\,U(x)\,\eta(x) + \cos(U(x))\,\eta(x) + \partial_x\,\eta(x)$$

3. *Example from Classical Mechanics:* $EL(q)(t) := -\,\ddot{q}(t) - q(t) + 3\,q(t)^2$

$$lin(EL, q, v, t) = -\,\ddot{v}(t)) - v(t) + 6\,q(t)\,v(t)$$

Generalization: functions of more variables (Evolution Equations)
For instance, two variables.

Procedure lin2

```
lin2 := proc(F, u, v, t, x) local eps, line, dv;
line := eps- > unapply(U(t, x) + eps * V(t, x), (t, x));
dv := unapply(simplify(subs(eps = 0,
diff(F(line(eps))(t, x), eps))), (U, V, t, x));
dv(u, v, t, x);
end;
```

Exercise 165 *1.* $F(u)(t,x) := u(t,\, x)^2 + \sin(u(t,\, x))$

$$lin2(F, U, v, t, x) = 2\,U(t,\, x)\,v(t,\, x) + cos(U(t,\, x))\,v(t,\, x)$$

2. $G(u)(x,y) := (\partial_x\, u(x,\, y))^2 + (\partial_y\, u(x,\, y))^2 + x\,u(x,\, y)^2$

$$\begin{aligned} lin2(G, U, \eta, x, y) &= 2\,\partial_x\, U(x,\, y)\,\partial_x\,\eta(x,\, y)) \\ &\quad +2\,\partial_y U(x,\, y)\ \partial_y\,\eta(x,\, y)) + 2\,x\,U(x,\, y)\,\eta(x,\, y) \end{aligned}$$

3. Standard form of first-order Evolution Eqn: $Eq(u) = 0$ with vector field $K = K(u)$:

$$Eq(u)(t,x) := \partial_t\, u(t,\, x) - K(u)(t,\, x)$$

For instance, the KdV-eqn: $KdV(u)(t,x) := \partial_t\, u(t,\, x) - \partial_x^3\, u(t,\, x) - u(t,\, x)\,\partial_x\, u(t,\, x))$

$$\begin{aligned} lin2(KdV, U, \eta, t, x) &= \partial_t\,\eta(t,\, x) - \partial_x^3\,\eta(t,\, x) \\ &\quad -\eta(t,\, x)\,\partial_x\, U(t,\, x) - U(t,\, x)\,\partial_x\,\eta(t,\, x) \end{aligned}$$

4. In Maple there is a slightly different way to define the equation; actually it is more natural to start with the vector field K as being defined on the state space (as is the common way to view a vector field): $K_1(u)(x) := \partial_x^3\, u(x) + u(x)\,\partial_x\, u(x)$. Then the evolutionary map $t \mapsto u(t)$ becomes the argument of K_1, and we have

$$K_1(u(t))(x) = K(u)(t,x).$$

9.2 Variational derivative

9.2.1 Introduction theory

The first variation of the functional F at the point u in the direction v is a functional that is linear in v.

For a density functional (with density that depends on u and a finite number (N) of its derivatives), this linear functional when $N = 1$ is of the form

$$\int a_0(x)\,v(x) + a_1(x)\,\partial_x v(x))\,dx$$

and more generally

$$\int \sum_{k=0}^{N} a_k(x)\,\partial_x^k v(x)\,dx$$

where the coefficients $a_0(x), ...a_N(x)$ are expressions in u; the precise form is of no interest at this moment.

The *variational derivative* of F at the point u is defined to be that function, denoted by $\delta\, F(u)$, such that for all functions v that vanish (together with its derivatives) near the boundary points of the integral, it holds that:

$$\delta\, F(u,\, v) = \int \delta\, F(u)\, v(x)\, dx$$

In Maple-notation we write "varder(F,u)" for $\delta\, F(u)$.

By partial integration the variational derivative can be obtained from the first variation: if

$$fvar(F,\, u,\, v) = \int \sum_{k=0}^{N} a_k(x)\, \partial_x^k\, dx$$

then (partial integrations, neglecting possible boundary contributions):

$$fvar(F,\, u,\, v) = \int \sum_{k=0}^{N} [(-1)^k\, \partial_x^k[a_k(x)] \times v(x)\, dx$$

and hence the variational derivative is given by

$$varder(F,\, u) = \sum_{k=0}^{N} (-1)^k\, \partial_x^k[a_k(x)]$$

Formulated in this way, this is a clear procedure to obtain "varder"from "fvar". However, starting with a given functional, the coefficients a_k in ‘fvar’ are calculated (by Maple), and first have to be detected before we can write the expression for varder.
The procedure to do so is an iterative one on the density; the coefficients are recursevely obtained by substitution of powers of x for the function v.

9.2.2 Procedure

The ’student’ package allows one to detect the integrand from a given integral (provided the whole expression is under the integral sign); we modify the procedure ’fvar’ slightly for that aim.
Although that could be avoided, for computational simplicity (and without too much restriction) the procedure asks as input the order (N) of the highest derivative in the integrand of the functional, and the variable that is used in the description of the functional with ’int’.

Procedure varder
$varder \; := \; proc(F, u, N, x)$

```
local v, t, vd, a, k, n, m, eps, den, locffvar;
locffvar := unapply(subs(eps = 0,
diff(F(unapply(u(t) + eps * v(t), t)), eps)), v);
den := unapply(integrand(locffvar(v)), v);
a[0] := den(unapply(1, t));
vd := a[0];
for n from 1 to N do
a[n] := simplify(den(unapply(t^n/n!, t)) -
sum('a[k] * x^(n - k)/(n - k)!',' k' = 0..n - 1);
vd := vd + (-1)^n * Diff(a[n], xn); od;
vd;
end;
```

Exercise 166 *1.* $L(u) := \int_0^1 x\,u(x)^2 + (\frac{\partial}{\partial x}\,u(x))^2\,dx$

$$varder(L, u, 1, x) == 2\,x\,u(x) - 2\,(\frac{\partial^2}{\partial x^2}\,u(x))$$

2. $L(u) := \int_0^1 sin(x)\,u(x)^2 + x^3\,(\frac{\partial}{\partial x}\,u(x))^2\,dx$

3. $L(u) := \int u(x)^2 + (\frac{\partial}{\partial x}\,u(x))^2\,dx$

$$varder(L, u, 1, x) = 2\,u(x) - (\frac{\partial}{\partial x}\,(2\,(\frac{\partial}{\partial x}\,u(x))))$$

4. $H(u) := \int_0^1 \left[sin(u(x)) + (\frac{\partial^2}{\partial x^2}\,u(x))^2\right]\,dx$

$$varder(H, \psi, 2, x) = \cos(\psi(x)) - (\frac{\partial}{\partial x}\,0) + (\frac{\partial^2}{\partial x^2}\,(2\,(\frac{\partial^2}{\partial x^2}\,\psi(x))))$$

5. $K(u) := \int_0^1 \left[u(x)^4 + (\frac{\partial}{\partial x}\,u(x))^7\right]\,dx$

6. $J(u) := \int_0^1 n(x)\,\sqrt{1 + (\frac{\partial}{\partial x}\,u(x))^2}\,dx$

$$varder(J, u, 1, x) = -\left(\frac{\partial}{\partial x}\frac{n(x)\,(\frac{\partial}{\partial x}\,u(x))}{\sqrt{1 + (\frac{\partial}{\partial x}\,u(x))^2}}\right)$$

7. *Examples from Classical Mechanics*

(a) $L(q) := \int \left[\frac{1}{2}\,\dot{q}(t)^2 - \frac{1}{2}\,q(t)^2 + q(t)^3\right]\,dt$

$$varder(L, q, 1, t) = -q(t) + 3\,q(t)^2 - \ddot{q}(t)$$

(b) $L(q) := \int \left[\frac{1}{2}\,(\frac{\partial}{\partial t}\,q(t))^2 - U(q(t))\right]\,dt$

(c) $L(q) := \int Lag(q(t),\,\dot{q}(t))\,dt$

9.3 Second variation

The second variation of a functional F at a point u in a given direction v, denoted by $\delta^2 F(u,v)$ is nothing but the second derivative of the functional when restricted to the line in the given direction:

$$\delta^2 F(u,v) := \frac{d^2}{d\varepsilon^2} F(u+\varepsilon v)\bigg|_{\varepsilon=0}$$

This leads to a quadratic functional in v.
In Maple-notation we write Svar(F,u,v) for $\delta^2 F(u,v)$.

In a different way, the second variation can be obtained by repeated differentiation; this leads to a bilinear functional of two directions, that will be denoted by svar(F,u,v,w).

Procedures Svar(F,u,v) and svar(F,u,v,w)
$Svar\ :=$
$(G,u,v)->simplify(subs(eps=0,$
$diff(G(unapply(u(t)+eps*v(t),t)),eps\$2)));$

$svar\ :=$
$(G,u,v1,v2)->simplify(subs((eps=0,rho=0),$
$diff(G(unapply(u(t)+eps*v1(t)+rho*v2(t),t)),eps,rho))).$

The relation is as aspected from repeated differentiation:

$$Svar(F,\ u,\ v) = svar(F,\ u,\ v,\ v)$$

Exercise 167 *1.* $K := u \to \int u(x)^5\,dx$

$$svar(K,u,v,w) = 20\int u(x)^3\, v(x)\, w(x)\, dx$$

$$Svar(K,u,v) = 20\int u(x)^3\, v(x)^2\, dx$$

2. $F(u) := \int \left[\frac{1}{2}\,\partial_x\, u(x)^2 + x^3 \sin(u(x)) + u(x)^5\right]\, dx$

$$Svar(F,u,v) = \int \left[\partial_x\, v(x)^2 - x^3\, \sin(u(x))\, v(x)^2 + 20\, u(x)^3\, v(x)^2\right]\, dx$$

$$svar(F,u,v,w) = \int \left[\begin{array}{c} \partial_x\, w(x)\, \partial_x\, v(x)) - x^3\, \sin(u(x))\, w(x)\, v(x) \\ +20\, u(x)^3\, v(x)\, w(x) \end{array}\right] dx$$

9.4 Exercises

1. Consider the Euler-Lagrange equation of the action functional of the **harmonic oscillator**, which is the integral of kinetic minus potential energy:

   $$L := q \to \int \left[\frac{1}{2}\dot{q}^2 - \frac{1}{2}q^2\right] dt$$

   Determine the Lie-derivative of the total energy E along this vector field:

   $$E := q \to \frac{1}{2}\dot{q}^2 + \frac{1}{2}q^2$$

2. Show that the **KdV-eqn** can be written as a Hamiltonian system by determining the Hamiltonian H such that

   $$\partial_t\, u(t) = \partial_x\, \mathit{varder}(H,\, u,\, 1,\, x)$$

3. Show that the following functionals are constants of the motion for KdV: $\int u(x)\, dx$, $\int u(x)^2\, dx$, $H(u)$.

4. Show that the **BBM-eqn** can be written as a Hamiltonian system by determining the Hamiltonian H such that

   $$\partial_t\, u(t) = L\, \partial_x\, \mathit{varder}(H,\, u,\, 1,\, x)$$

   where L is the inverse of a suitable differential operator.

5. Show that the following functionals are constants of the motion for BBM: $\int u(x)\, dx$, $\int u(x)^2\, dx$, $H(u)$.

6. Show that **Burgers' eqn** can be written as a combination of a conservative and dissipative structure by determining the functionals D and Hsuch that

   $$\partial_t\, u(t) = \partial_x\, \mathit{varder}(H,\, u,\, 1,\, x)) + \mathit{varder}(D,\, u,\, 1,\, x)$$

   Can you find an alternative way to describe the dissipative part?

7. Determine the structure of the **reaction-diffusion eqn** .

8. **Transformation:** Consider an evolution equation (in finite dimensions for simplicity) of the general form

   $$\partial_t\, u(t) = M\, \mathit{grad}(E(u),\, u)$$

   where M is a square matrix, and E a function on state space.

   Determine the equation for v that is related to u by the linear transformation $v = T\, u$.

   Show that if the equation for u is a conservative (or gradient) system, the same holds for the equation for v.

9. **Linearization:** determine the linearization of
   a. the KdV-eqn around the trivial state
   b. the Burgers'-eqn around a constant solution
   c. the KdV-eqn around a soliton solution
   d. the Burgers-eqn around a front solution

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