# Variational Methods

supporting text for Lectures on Mathematical Optics

(synopsis from Lecture Notes 'Applied Analytical Methods' 150950)

E. van Groesen
(groesen@math.utwente.nl)

Applied Analysis & Mathematical Physics
Faculty of Mathematical Sciences

University of Twente

January 2001

POBox 217,
7500 AE Enschede
The Netherlands

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# Chapter 1

# Introduction

In these notes 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.
Below we present a brief overview of the contents of the notes.

## 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

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

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:
>
> $$f'(\hat{x}) = 0.$$

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 $\nabla F$ 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 $\eta$ is found by differentiating the scalar function obtained by restricting $F$ to the line through $x$ in the direction $\eta$, 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 $\eta$:

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

From $\nabla F(x) \cdot \eta = 0$ for all $\eta$, 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)
>
> *"..... des loix du mouvement ou l'action est toujours employee avec la plus grande economie, demontreront l'existence de l'Etre supreme ... "*, (Maupertuis, 1757)
>
> **Fermat's principle**[1], 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.

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

[1] 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.

found in the seventeenth century. From a more closer historical investigation it becomes clear that practical problems from physics provided the initial motivation for the beautiful mathematical theory that has been developed since then.

## 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. The systems referred to above, Lagrangian and Hamiltonian systems, often have special (but important)solutions which 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.

# 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 definitions and properties for linear and quadratic functionals are summarized.

### 2.1.1 Notation, function spaces

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

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

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 $u, v \in \mathcal{U}$

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

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 $\Omega$.

### 2.1.2 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 restrictions of the functions in the interior of the domain $\Omega$. 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 $\eta$, for each test function $\eta$, belongs completely to the set of admissible elements:

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

### 2.1.3 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 $u$, all tangent vectors at $u$ obtained as derivatives of curves on $\mathcal{M}$ through $u$ (see

Fig. 2.1). 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

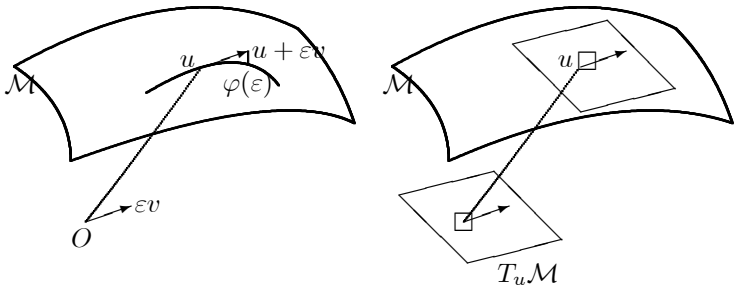


Figure 2.1: A tangent vector $v$ to the manifold $\mathcal{M}$ at a point $u$ defines a line that is tangent to a curve on $\mathcal{M}$,; the set of such tangent vectors defines the tangent space $T_u\mathcal{M}$ at $u$.

In the 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 $\varepsilon$.

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

**Definition 1** *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.

### 2.1.4 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 $\mathcal{L}$.

**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.

[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

**Example 2** *Single integral functionals*
When the domain of definition of the functions is an interval ($m = 1$), the functionals are called single integral functionals. For instance, 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 $\mu$ and $\sigma$ are certain material functions, and $f$ an applied force.

**Example 3** *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

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

### 2.1.5 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 $\Omega$ and its derivatives (not necessarily derivatives along the boundary!):

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

### 2.1.6 Bilinear functionals and quadratic forms

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

A functional $\ell$ 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

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

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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.

A bilinear functional $b$ can have special properties:

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

Note the following fact:

$b(u,u) = 0$ if $b$ 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 4** *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 5** *For the symmetric bilinear functional $b$ and the corresponding quadratic form $a$, the following relations hold:*

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

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

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

## 2.2 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.

### 2.2.1 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 6** 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*

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

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 $\varepsilon$: $o(\varepsilon)/\varepsilon \mapsto 0$ 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.

[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:

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

**Definition 7** *The function $\delta\mathcal{L}(u)$ on $\Omega$ defined by the condition*

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

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

It will follow from Lagrange's Lemma 11 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.

### 2.2.2 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 $\varepsilon$.

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

**Definition 8** *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:*

$$\delta\mathcal{L}(\hat{u};v)=0\ \ \textit{for all } v\in T_{\hat{u}}\mathcal{M}. \tag{2.6}$$

*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 9** *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": *(2.6) 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.*

### 2.2.3 Euler-Lagrange equation for unconstrained problems

It is possible to translate condition (2.6) 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 (2.6) and the fact that $T_u\mathcal{M}\supset C_0^\infty(\Omega)$, it follows that certainly it must hold that

$$\delta\mathcal{L}(\hat{u};\eta)\equiv\langle\delta\mathcal{L}(\hat{u}),\eta\rangle=0\ \ \text{for all } \eta\in C_0^\infty(\Omega). \tag{2.7}$$

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

**Proposition 10** 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*

$$\delta\mathcal{L}(\hat{u}) = 0. \tag{2.8}$$

*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 (2.7) and the following basic Lemma.

**Lemma 11** Lagrange's Lemma
*Let $f$ be a continuous function on $\Omega$ that is such that*

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

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

### 2.2.4 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:

$$\int_{\partial\Omega} b(\hat{u}; v) = 0, \quad \text{for all} \quad v \in T_{\hat{u}}\mathcal{M}. \tag{2.9}$$

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 (2.6) itself.

## 2.3 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 12** *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*

$$\delta^2\mathcal{L}(u; v) = \frac{d^2}{d\varepsilon^2}\mathcal{L}(u + \varepsilon v)\bigg|_{\varepsilon=0}. \tag{2.10}$$

Hence we have

$$\mathcal{L}(u + \varepsilon v) = \mathcal{L}(u) + \varepsilon\delta\mathcal{L}(u; v) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{L}(u; v) + o(\varepsilon^2). \tag{2.11}$$

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

**Proposition 13** *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 $\bar{u}$:*

$$\mathcal{L}(\bar{u}) \leq \mathcal{L}(u) \text{ for all } u \in \mathcal{M} \quad \text{in a neighbourhood of } \bar{u}, \tag{2.12}$$

*then*

$$\delta^2\mathcal{L}(\bar{u}; v) \geq 0 \text{ for all } \quad v \in T_{\bar{u}}\mathcal{M}. \tag{2.13}$$

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:

$$Q(u; v, w) := \frac{d}{d\rho}\frac{d}{d\varepsilon}\mathcal{L}(u + \varepsilon v + \rho w)\Big|_{\varepsilon=0,\rho=0}. \tag{2.14}$$

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

$$Q(u; v, w) = Q(u; w, v) \tag{2.15}$$

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

$$Q(u; v, w) = \int_\Omega v \cdot Q(u)w \equiv \langle v, Q(u)w\rangle. \tag{2.16}$$

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

$$\delta^2\mathcal{L}(u; v) = \langle v, Q(u)v\rangle, \tag{2.17}$$

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 14** *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 $D\delta\mathcal{L}$:*

$$D\delta\mathcal{L}(u)\xi := \frac{d}{d\varepsilon}\delta\mathcal{L}(u + \varepsilon\xi)\Big|_{\varepsilon=0}. \tag{2.18}$$

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

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

## 2.4 Variational structures in nature and dynamics

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.

### 2.4.1 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 $\gamma$ 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 15** *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.* 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 $\theta$ according to

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

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.

### 2.4.2 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 $\phi$. In the presence of a charge distribution $\rho$ 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 $\tau$; 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 $\phi$ 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 16** *1.* Show that a critical point of

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

satisfies

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

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 $\psi_2$ and $\rho$ 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?

### 2.4.3 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.

#### 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 17** *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

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

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

$$\mathcal{A}(q) = \int_{t_0}^{t_1} L[q](t) dt. \tag{2.19}$$

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

$$-\frac{d}{dt}[L_v[q]] + L_q[q] = 0. \tag{2.20}$$

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

$$L(q, v) = \frac{1}{2} v \cdot Mv - V(q) \tag{2.21}$$

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

$$\frac{d}{dt}[M\dot{q}] = -\partial_q V(q). \tag{2.22}$$

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 $\Omega_0$, i.e. $V(u) = \int_{\Omega_0} W[u]dx$. Then take as action functional the difference of kinetic and potential energy:

$$\mathcal{A}(u) = \int dt[\int_{\Omega_0} \frac{1}{2}\rho(x)u_t^2 dx - V(u)]. \tag{2.23}$$

The Euler-Lagrange equation can be written as

$$\rho(x)\partial_t^2 u = -\delta_u V(u) \tag{2.24}$$

where $\delta_u V(u)$ denotes the variational derivative of $V$ with respect to functions on the spatial domain $\Omega_0$.
For instance, for the specific choice ($\sigma$ is a given positive function on $\Omega_0$, and $f$ a given function depending on $u$ and possibly $x$)

$$V(u) = \int (\frac{1}{2}\sigma(x)|\nabla u|^2 + f(u)), \tag{2.25}$$

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

$$\rho(x)\partial_t^2 u = \text{ div }(\sigma(x)\nabla u) - \frac{df(u)}{du}. \tag{2.26}$$

This is a (nonlinear) wave equation. When, $\rho$ and $\sigma$ 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 $\Delta$ the Laplace operator.

### Hamiltonian systems

Hamiltonian systems are systems that can also be found from a variational principle: the *canonical action principle*.
With $q \in Q$ ("position") and $p$ ("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:

$$H = H(t, q, p).$$

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 18** *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

$$\begin{cases} \partial_t q &= \frac{\partial H}{\partial p} \\ \partial_t p &= -\frac{\partial H}{\partial q} \end{cases} \tag{2.27}$$

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

**Example 19** As a specific example of a finite dimensional system, verify that Newtons equations as given above, are also obtained for

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

**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 20** *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:*

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

*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:*

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

*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.

## 2.5 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.

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

   Derive the corresponding expressions for the second variation.

2. *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.

   (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 $-\infty$.

3. *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 21** *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 $\delta^2\mathcal{L}(u;\cdot)$.*

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.

# Chapter 3

# Constrained variational problems

## 3.1 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 $\mathcal{K}_1, \ldots, \mathcal{K}_p$:

$$\mathcal{M} \;=\; \{\; u \in \mathcal{U} \;\mid\; \mathcal{K}_1(u) = k_1, \ldots, \mathcal{K}_p(u) = k_p \;\}, \tag{3.1}$$

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 $\mathcal{M}$.

### 3.1.1 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 22** *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 23** *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 $L_2(\Omega)$)*

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

### 3.1.2 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 24** *(Lyusternik)*
*The* tangent space *to $\mathcal{M}$ at a regular point $u \in \mathcal{M}$ is the set*

$$T_u\mathcal{M} := \{\ v \in \mathcal{U}_0 \ \mid\ \delta\mathcal{K}_1(u;v) = \ldots = \delta\mathcal{K}_p(u;v) = 0\ \}. \tag{3.2}$$

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.

## 3.2 Lagrange's multiplier rule

Recall the general stationarity condition (2.6) 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

$$\begin{aligned} \delta\mathcal{L}(\hat{u}; v) = 0, \quad & \text{for all} \quad && v \in \mathcal{U}_0 \\ & \text{for which} \quad && \delta\mathcal{K}_k(\hat{u}; v) = 0, 1 \leq k \leq p. \end{aligned} \tag{3.3}$$

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, (3.3) 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 25** 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 (3.3), if and only if there are real numbers, called* Lagrange multipliers, *$\lambda_1, \ldots, \lambda_p$ such that*

$$\delta\mathcal{L}(\hat{u}; v) = \sum_k \lambda_k \delta\mathcal{K}_k(\hat{u}; v), \quad \textit{for all} \quad v \in \mathcal{U}_0. \tag{3.4}$$

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

**Proposition 26** *A regular point $\hat{u} \in \mathcal{M}$ is a critical point of $\mathcal{L}$ on the constrained set $\mathcal{M}$ (3.1) iff for some multipliers $\lambda_1, \ldots, \lambda_p$ the element $\hat{u}$ is an* unconstrained *critical point of the* unconstrained *functional*

$$\mathcal{U} \ni u \mapsto \mathcal{L}(u) - \sum_m \lambda_m \mathcal{K}_m(u). \tag{3.5}$$

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

This result has an obvious consequence for the relation between the variational derivatives since $C_0^\infty \subset \mathcal{U}_0$. When no natural boundary conditions appear, the 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 (3.4).

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

**Proposition 27** *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.*

## 3.3 Constrained Second Variation

For the manifold $\mathcal{M}$ given in (3.1) we calculate the second variation at a constrained critical point $\hat{u}$ that satisfies (3.4).
To that end, take $v \in T_{\hat{u}}\mathcal{M}$ and investigate for which functions $w$, depending on $\varepsilon$ 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

$$\begin{aligned} \mathcal{K}(\hat{u} + \varepsilon v + w) &= \mathcal{K}(\hat{u}) + \delta\mathcal{K}(\hat{u}; \varepsilon v + w) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{K}(\hat{u}; v) + o(\varepsilon^2) \\ &= \mathcal{K}(\hat{u}) + \delta\mathcal{K}(\hat{u}; w) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{K}(\hat{u}; v) + o(\varepsilon^2) \end{aligned} \tag{3.6}$$

that $w$ has to satisfy

$$\delta\mathcal{K}_k(\hat{u}; w) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{K}_k(\hat{u}; v) + o(\varepsilon^2) = 0, \tag{3.7}$$

for $1 \leq k \leq p$. Calculating the functional $\mathcal{L}$ on such a curve, using equation (3.4) for $\hat{u}$, produces

$$\begin{aligned} &\mathcal{L}(\hat{u} + \varepsilon v + w) \\ &\quad = \mathcal{L}(\hat{u}) + \varepsilon\delta\mathcal{L}(\hat{u}; v) + \delta\mathcal{L}(\hat{u}; w) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{L}(\hat{u}; v) + o(\varepsilon^2) \\ &\quad = \mathcal{L}(\hat{u}) + \sum_k \lambda_k \delta\mathcal{K}_k L(\hat{u}; w) + \frac{1}{2}\varepsilon^2\delta^2\mathcal{L}(\hat{u}; v) + o(\varepsilon^2). \end{aligned} \tag{3.8}$$

Inserting the expression for $\delta\mathcal{K}_k(\hat{u}; w)$ from (3.7), there results:

$$\begin{aligned} &\mathcal{L}(\hat{u} + \varepsilon v + w) = \\ &\qquad \mathcal{L}(\hat{u}) + \frac{1}{2}\varepsilon^2 \left[\delta^2\mathcal{L}(\hat{u}; v) - \sum_k \lambda_k \delta^2\mathcal{K}_k(\hat{u}; v)\right] + o(\varepsilon^2) \end{aligned} \tag{3.9}$$

The expression

$$\delta^2\mathcal{L}(\hat{u}; v) - \sum_k \lambda_k \delta^2\mathcal{K}_k(\hat{u}; v) \tag{3.10}$$

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 (3.5) that leads to the equation for $\hat{u}$, but restricted to variations form the tangent space.

**Proposition 28** *If $\bar{u}$ is a local extremal for $\mathcal{L}$ on the manifold $\mathcal{M}$ given by (3.1), that satisfies the multiplier equation (3.4), the constrained second variation (3.10) is sign-definite in all directions $v$ from the tangent space.*
*Specifically, if $\mathcal{L}$ has a (local) minimum at $\bar{u}$, then*

$$\delta^2\mathcal{L}(\bar{u};v) - \sum_k \lambda_k \delta^2\mathcal{K}_k(\bar{u};v) \geq 0 \text{ for all } v \in T_{\bar{u}}\mathcal{M}. \tag{3.11}$$

## 3.4 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 $I$:

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

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 $\gamma$. Now we will treat $\gamma$ 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 $\gamma$ in a neighbourhood of some $\gamma_0$. It may happen that, for instance, this family consists only of constrained minimizers, but also that the character of the critical point changes with $\gamma$ (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

$$n(U) := \frac{dU}{d\gamma}, \tag{3.12}$$

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

$$\langle \delta I(U), n(U) \rangle = 1. \tag{3.13}$$

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

$$\delta H(U(\gamma)) = \lambda(\gamma)\delta I(U(\gamma)). \tag{3.14}$$

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

**Definition 29** *The* value function *of the constrained critical point problem on a branch of critical points is defined as:*

$$h(\gamma) := H(U(\gamma)) = \textit{Crit } \{H(u) \mid I(u) = \gamma\}. \tag{3.15}$$

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 $\gamma$, a schematic representation of these equilibria in the integral diagram may look like Fig. 3.1.

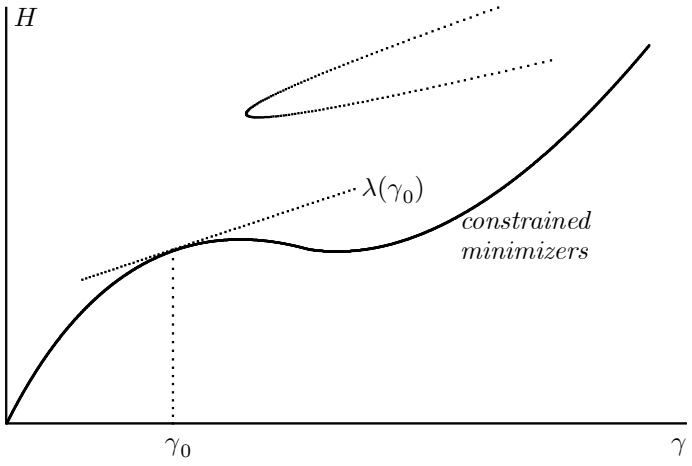


Figure 3.1: The integral diagram. Schematic presentation of the value function of the constrained minimization problem (solid line). No states correspond to points below this solid line. The tangent to this curve has slope $\lambda(\gamma)$. Other curves (dotted) represent branches of relative equilibria 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.

### 3.4.1 The multiplier as derivative of the value function

**Proposition 30** *For the smooth family $\gamma \mapsto U(\gamma)$, the multiplier $\lambda(\gamma)$ appearing in (3.14) is related to the value function according to*

$$\lambda(\gamma) = \frac{dh(\gamma)}{d\gamma}. \tag{3.16}$$

**Proof.** A direct differentiation with respect to $\gamma$ 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 $\gamma_0$ as being embedded in a family provides an interpretation of the Lagrange multiplier $\lambda(\gamma_0)$.

The character of the constrained critical point at $\gamma_0$ 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, actually the conexity or concavity of the value function.

**Proposition 31** *A constrained minimizer of $H$ on level set of $I$ is an unconstrained (local) minimizer of $H - \lambda I$ (where $\lambda$ 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 $H - \lambda I$. See Fig. 3.2.*

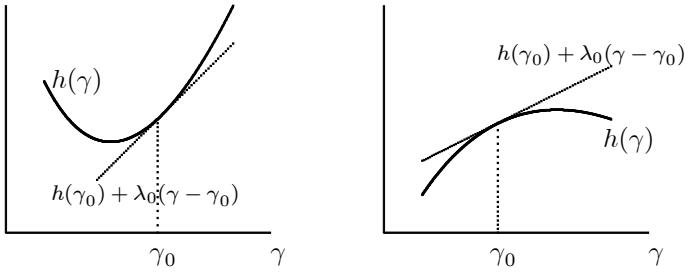


Figure 3.2: With the bold line the graph of the value function $h$, the tangent to this graph at $\gamma_0 : \gamma \mapsto h(\gamma_0) + \lambda_0(\gamma - \gamma_0)$, lies below this graph if $h$ is locally convex (at the left), or above this graph if $h$ is locally concave (at the right). In the convex 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 $H - \lambda_0 I$.

## 3.5 Relative Equilibria

In this section we briefly describe the main ideas and some examples how constrained problems appear in dynamical systems.
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) is described e.g. 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

   $$-I''(u_0)J\delta H(u_0) = \delta H(u_0) \quad \text{for all } u_0.$$

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 $\phi$. 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.*

**Example 32** 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).

**Exercise 33** *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 $\partial_x$. Show that the Hamiltonian is conserved as a consequence of the skew-symmetry of $\partial_x$.

*2.* A *travelling wave* is a solution of the form

$$t \mapsto U(x - \lambda t);$$

here $U$ is the waves shape and $\lambda$ 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 $\lambda$) 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.

## 3.6 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

$$\begin{aligned} \text{Crit } \{\mathcal{K}(x) \mid \mathcal{V}(x) &= R, x \in X\}, \\ \text{with } \mathcal{K}(x) &= \int_0^1 \frac{1}{2}|\dot{x}|^2 d\tau, \quad \mathcal{V}(x) = \int_0^1 V(x) d\tau \end{aligned}$$

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. *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 $2\pi$ 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 $\gamma$ 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 4

# 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 $\lambda_p$ of this algebraic equation with *algebraic multiplicity* $\alpha_p$ 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. 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 compariosn arguments, and numerical procedures to calulate non-principal eigenvectors and eigenvalues, non-successive characterizations are very usefull, and will be considered also.

## 4.1 Formulation, examples

### 4.1.1 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 $\lambda$ 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 $\Omega$.

**Definition 34** *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

$$b(u, v) := < Lu, v > .$$

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

$$\delta \mathcal{Q}(u; v) = 2b(u, v) \text{ for all } u, v \in \mathcal{U}$$

In the following we will mainly deal with differential operators.

**Example 35** *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.

**Exercise 36** *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 $a, b_1, \ldots, b_n, c$, 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 37** *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 38** *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*

$$\mathcal{Q}(u) = \int_\Omega [p(x)|\nabla u|^2 + q(x)u^2]dx.$$

### 4.1.2 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 $E_\lambda$.
First the result that can be expected for symmetric operators.

**Proposition 39** *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:*

$$\text{for } \varphi \in E_\lambda,\ \psi \in E_\mu, \text{ with } \lambda \neq \mu \quad \begin{cases} \mathcal{Q}(\varphi,\psi) &= 0 \\ \mathcal{N}(\varphi,\psi) &= 0. \end{cases}$$

*We can denote this for the eigenspaces as*[1]

$$E_\lambda \perp_{\mathcal{N}} E_\mu, \quad E_\lambda \perp_{\mathcal{Q}} E_\mu \text{ when } \lambda \neq \mu.$$

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 $\lambda$:

$$\mathcal{Q}(\varphi, v) = \lambda \mathcal{N}(\varphi, v) \quad \textit{for all} \;\; v \in \mathcal{U}.$$

Since this can be rewritten like

$$\delta\mathcal{Q}(u; v) = \lambda \delta\mathcal{N}(u; v),$$

[1] 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.

one interpretation of an eigenfunction with eigenvalue $\lambda$ is as a critical point of the functional

$$\mathcal{U} \ni u \to \mathcal{Q}(u) - \lambda \mathcal{N}(u).$$

However, since $\lambda$ is not given, but has to be found, this is not a very useful attack. Much more fruitful is to interpret $\lambda$ as a multiplier appearing from a constrained problem.

**Proposition 40** *(Normalized) Eigenfunctions $\varphi$ are critical points of:*

$$\varphi \in \{\mathcal{Q}(u) \,|u \in U,\ \mathcal{N}(u) = 1\}.$$

*Equivalently,*

$$\varphi \in \{\mathcal{R}(u) \,|u \in U\}, \textit{ with } \mathcal{R}(u) = \frac{\mathcal{Q}(u)}{\mathcal{N}(u)}.$$

*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 $\gamma \in \mathcal{R}$

$$\mathcal{R}(u) \geq \gamma, \textit{ and for some sequence } u_m,\ \mathcal{R}(u_m) \to \infty.$$

## 4.2 Spectral theorem for symmetric differential operators

**Theorem 41** 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*

$$\varphi_1 \in Min\ \{\mathcal{Q}(u) \quad |u \in \mathcal{U},\ \mathcal{N}(u) = 1\} \sim Min\,\{\mathcal{R}(u) \,|u \in \mathcal{U}\}$$

*is the* principal eigenfunction $\varphi_1$*, i.e. the eigenfunction corresponding to the smallest eigenvalue, the* principal eigenvalue*, $\lambda_1$ that is given by*

$$\lambda_1 = \mathcal{R}(\varphi_1)\ (\geq \gamma).$$

Any other eigenfunction (independent of $\varphi_1$) can be assumed to be orthogonal (both in $\mathcal{N}$-, as well as in $\mathcal{Q}$-sense) to $\varphi_1$. In the following formulation this will be exploited in a successive way.

**Theorem 42** 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"* $\lambda_k$ *in the sense that* $\lambda_{k+1} \geq \lambda_k$*, while, when* $\lambda_{k+1} > \lambda_k$*, there are no other eigenvalues inbetween.*

**Remark 43** *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 $\mu, \sigma$

$$L\psi = \mu N\psi + \sigma f, \quad \text{with} \quad \mu = \mathcal{R}(\psi).$$

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 $\lambda_{k+1}$ 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 $\lambda_1$, an error in the calculation of $\varphi_1$ influences the constraint set for $\lambda_2$ and induces an additional error in the calculation of $\lambda_2$ and of $\varphi_2$, 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 $\varphi_1$ is constructed that is correct up to order $\varepsilon$ (in $\mathcal{N}$-norm for instance): $\varphi_1 - \hat{\varphi}_1 = \mathcal{O}(\varepsilon)$.Then the approximate first eigenvalue $\hat{\lambda}_1$ that is constructed is correct up to order $\varepsilon^2$: $\lambda_1 - \hat{\lambda}_1 = \mathcal{O}(\varepsilon^2)$.

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 $\mathcal{N}$.

**Theorem 44** 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.*

**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

$$\mathcal{N}(u - \sum_1^M u_m \varphi_m) \to 0 \quad for\ \ M \to \infty$$

and also in the stronger norm

$$\mathcal{Q}(u - \sum_1^M u_m \varphi_m) \to 0 \quad for\ \ M \to \infty.$$

**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 $\lambda_m$ are non-zero (the operator $L$ is invertible),
- *or*, if there is a zero eigenvalue, with eigenspace $E_{\lambda=0}$ *(*consisting of the eigenfunctions with eigenvalue 0*)*,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.

### 4.2.1 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 $\rho$ 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

$$\mathcal{N}(u) = \int \rho(x)u^2, \quad \mathcal{Q}(u) = \int [p(x)u_x^2 + q(x)u^2].$$

**Example 45** *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

$$|u|_\infty^2 \leq c_1 \int u_x^2 \quad \text{for all } u,\ u(0 = u(\pi) = 0.$$

Then the convergence in the $Q$-norm implies the *pointwise* convergence of the Fourier-sine series:

$$|u - \sum_1^M u_m\varphi_m(x)|_\infty \to 0, \ \text{for} M \to \infty.$$

**Exercise 46** *1.* 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.

*2.* 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.*

**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

$$\begin{aligned} -\text{div}\ (p(x)\nabla\phi) + q(x)\phi &= \lambda\phi \ \text{ in } \ \Omega \\ \phi &= 0 \quad \text{on } \partial\Omega_D \\ p(x)\partial_n\phi &= 0 \quad \text{on } \partial\Omega_N \end{aligned}$$

Sufficient conditions on the functions $p, \rho$ 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.

**Example 47** In a few specific cases, for special domains $\Omega$, 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

$$\begin{aligned} -\Delta\phi &= \lambda\phi \ \ in \ \ \Omega \\ \phi &= 0 \quad on\ \partial\Omega_D \\ \partial_n\phi &= 0 \quad on\ \partial\Omega_N \end{aligned}$$

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 $\Omega$. 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

$$\begin{aligned}\mathcal{N}(u) &= \int u^2 r dr d\phi \\ \mathcal{Q}(u) &= \int [u_r^2 + \tfrac{1}{r^2} u_\phi^2] r dr d\phi\end{aligned}$$

and the eigenvalue problem reads

$$\begin{aligned}-\Delta u &\equiv -\left[\frac{1}{r}\partial_r\left(r\partial_r u\right) + \frac{1}{r^2}\partial_\phi^2 u\right] = \lambda u, \quad \textit{for } r < 1 \\ u &= 0 \quad \textit{for } r = 1\end{aligned}$$

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 $\alpha$

$$-\partial_\phi^2\Phi = \alpha\Phi, \ \text{ and} - \frac{1}{r}\partial_r(rV_r) + \frac{\alpha}{r^2}V(r) = \lambda V.$$

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 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 $\lambda$ 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

$$\psi_{m,\ell} = J_m(\sigma_{m,\ell}r)\ [a\sin m\phi + b\cos m\phi], m \geq 0, \ell \geq 1.$$

3. *Special case: Radially symmetric solutions*
Consider the eigenfunctions that are independent of the angle variable $\phi$:

$$\lambda_{0,\ell} = \sigma_{0,\ell}^2, \quad \psi_{0,\ell} = J_0(\sigma_{0,\ell}), \ell \geq 1.$$

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

$$\int_0^1 J_0(\sigma_{0,k}r)J_0(\sigma_{0,m}r)rdr = 0, \quad \text{for} \quad k \neq m.$$

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

$$v_\ell = \frac{\int v(r)J_0(\sigma_{0,\ell}r)rdr}{\int J_0(\sigma_{0,\ell}r)^2 rdr}.$$

The convergence is with respect to the $\mathcal{N}_0$ and the $\mathcal{Q}_0$-norm.

## 4.3 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.

**Proposition 48** *Let $\mathcal{U}$ be the linear space, and $\mathcal{R}$ the Rayleigh quotient. Suppose that the principal eigenvalue $\Lambda$ minimizes $\mathcal{R}$ on $\mathcal{U}$; making its dependence explicitly, we write*

$$\Lambda(\mathcal{R},\mathcal{U}) = Min\{\mathcal{R}(u) \,|u \in \mathcal{U}\}$$

*Then $\Lambda$ 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

$$\mathcal{R}_1(u) \leq \mathcal{R}_2(u) \quad \textit{for all} \quad u \in \mathcal{U}$$

$$\Longrightarrow \text{ Min } \{\mathcal{R}_1(u)|u \in \mathcal{U}\} \leq \mathcal{R}_2(u) \quad \textit{for all} \quad u \in \mathcal{U}$$

$$\Longrightarrow \text{ Min } \{\mathcal{R}_1(u)|u \in \mathcal{U}\} \leq \text{Min } \{\mathcal{R}_2(u)|u \in \mathcal{U}\}.$$

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 ..."). □.

**Example 49** 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 $\Omega$ with the same boundary conditions. If

   $$p_1 \leq p_2, \quad q_1 \leq q_2, \quad \rho_1 \geq \rho_2 \quad \textit{on} \quad \Omega,$$

   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 $\Omega$, 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

$$\mathcal{U}_{1,2} = \{ \ u \ \mid \ u = 0 \ on \ \partial\Omega_{1,2} \ \}.$$

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 $\Omega_1$ by assigning it the value zero for $x \in \Omega_1/\Omega_2$; this defines the space of functions $\bar{\mathcal{U}_1} = \{ \ v : \Omega_1 \ \mid \ v = 0 \ for x \in \Omega_1/\Omega_2 \ \}$. 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

$$\begin{aligned} \Lambda_2 &= \text{Min } \{\mathcal{R}(v_2) |\ v_2 \in \mathcal{U}_2\} = \text{Min } \{\mathcal{R}(v_1) |\ v_1 \in \mathcal{U}_1\} \\ &\geq \text{Min } \{\mathcal{R}(u) |\ u \in \mathcal{U}_1\} = \Lambda_1 \end{aligned}$$

## 4.4 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.

### 4.4.1 Min-max and Max-Min formulations

**Formulation and notation**
Starting point are the quadratic forms $\mathcal{N}$ and $\mathcal{Q}$, and the eigenvalues $\lambda_k$ and eigenfunctions $\varphi_k$ 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 $n \in IN$ 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 50** *The eigenvalues $\lambda_{n+1}$ are found from the following non-successive characterizations:*

- Weyl-Courant characterization

  $$\lambda_{n+1} = Max\ \left\{ Min\ \{\mathcal{R}(u)|\ u \in \mathcal{U} \cap \mathcal{W}_n^{\perp}\}\right|\ \ \mathcal{W}_n\};$$

  *the maximum is attained for the choice $\mathcal{W}_n = \text{span}\{\varphi_1, \ldots, \varphi_n\}$ (a set of $n$ independent eigenfunctions with eigenvalue $\leq \lambda_n$), and for that choice, the minimum is attained for an eigenfunction $\varphi_{n+1}$ that has eigenvalue $\lambda_{n+1}$;*

- 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 $\mathcal{U}_{n+1} = \text{span}\{\varphi_1, \ldots, \varphi_n, \varphi_{n+1}\}$ (a set of $n+1$ independent eigenfunctions with eigenvalue $\leq \lambda_{n+1}$), and for that choice, the maximum is attained for an eigenfunction $\varphi_{n+1}$ that has eigenvalue $\lambda_{n+1}$.*

### 4.4.2 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 51** *Let $\mathcal{U}$ be the linear space, and $\mathcal{R}$ the Rayleigh quotient, and let theiegenvalues be found from the Weyl-Courant or the Poincaré characterization. Suppose that the eigenvalues $\lambda_n$ 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 $\lambda_n$ 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 $\mathcal{U}_1 \supset \mathcal{U}_2$.

# Chapter 5

# Annex: 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 MAPLE mws we deal with the **first variation** (directional derivative) and the **variational derivative** ( the "gradient" of a functional) of density functionals to illustrate the algebraic manipulations of the basic calculational aspects.

## 5.1 First variation

### 5.1.1 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)

$$\delta F(u, v) := \frac{d}{d\varepsilon} F(u + \varepsilon v)\Big|_{\varepsilon=0}.$$

**In Maple-notation we write "fvar(F,u,v)" for $\delta F(u, v)$.**

Note that $\varepsilon \rightarrow u + \varepsilon\, v$ 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*:

$$line := \varepsilon \rightarrow unapply(u(t) + \varepsilon\, v(t),\, t)$$

and the functional evaluated on this line

$$F(t \rightarrow u(t) + \varepsilon\, v(t))$$

has to be differentiated with respect to $\varepsilon$.
In one procedure,with some precautions for general use:

**Procedure fvar**
$fvar := proc\,(F,\,u,\,v)$
$local\ fv,\,\varepsilon;$
$fv := unapply(simplify(subs(\varepsilon = 0,$
$diff(F(unapply(U(\tau) + \varepsilon V(\tau),\,\tau)),\,\varepsilon))),\,U,\,V)\,;$
$fv(u,\,v)$
$end;$

This leads to the result that we want.

**Example 52** *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 :
$G := u \to \int \left[(\partial_x^2 u(x))^2 + u(x)^4\right]\,dx,$
$fvar(G,u,v) = 2\int (\frac{\partial^2}{\partial x^2}\,u(x))\,(\frac{\partial^2}{\partial x^2}\,v(x)) + 2\,u(x)^3\,v(x)\,dx$

**Exercise 53** *1.* 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)* $L := q \to \int \left[\frac{1}{2}\,\dot{q}^2 - U(q(t))\right]\,dt$

## 5.2 Variational derivative

### 5.2.1 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 $v$.

### 5.2.2 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;
```

**Example 54** *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. $L(u) := \int u(x)^2 + (\frac{\partial}{\partial x}\, u(x))^2\, dx$,
   $varder(L, u, 1, x) = 2\, u(x) - (\frac{\partial}{\partial x}\, (2\, (\frac{\partial}{\partial x}\, u(x))))$

3. $J(u) := \int_0^1 n(x) \sqrt{1 + (\frac{\partial}{\partial x}\, u(x))^2}\, dx$,
   $varder(J, u, 1, x) = -\frac{\partial}{\partial x} \frac{n(x)\, (\frac{\partial}{\partial x}\, u(x))}{\sqrt{1+(\frac{\partial}{\partial x}\, u(x))^2}}$

4. *Examples from Classical Mechanics*

**Exercise 55** 1. (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) $L(q) := \int \left[\frac{1}{2}\, (\frac{\partial}{\partial t}\, q(t))^2 - U(q(t))\right]\, dt$

## 5.3 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:

$$\delta^2 F(u, v) := \left.\frac{d^2}{d\varepsilon^2} F(u + \varepsilon v)\right|_{\varepsilon=0}$$

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:

$$Svar(F,\, u,\, v) = svar(F,\, u,\, v,\, v)$$

**Example 56** $K := u \to \int u(x)^5\, dx$,
$svar(K, u, v, w) = 20 \int u(x)^3\, v(x)\, w(x)\, dx$,
$Svar(K, u, v) = 20 \int u(x)^3\, v(x)^2\, dx$

# Bibliography


[1] V.I. Arnol'd, *Mathematical methods of classical mechanics*, Springer 1989 (revised edition).

[2] C. Carathéodory, *Calculus of Variations and partial differential equations*, Chelsea, New York, 1982.

[3] F.H. Clarke, *Optimization and nonsmooth analysis*, Wiley, New York, 1983.

[4] R. Courant & D. Hilbert, *Methods of Mathematical Physics*, vol 1, 2; Interscience Publishers, New York, 11953, 1962.

[5] I. Ekeland, *Convexity methods in Hamiltonian Mechanics*, Springer, Berlin, 1990.

[6] I. Ekeland and R. Temam, *Convex analysis and variational problems*, North-Holland, Amsterdam, 1976.

[7] B.A. Finlayson, *The method of weigthed residuals and variational principles*, Academic Press, New York, 1972.

[8] A. Friedman, *Variational principles and free boundary problems*, Wiley, New York, 1982.

[9] I.M. Gelfand & S.V. Fomin, *Calculus of Variations*, Prentice Hall, 1963.

[10] H. Goldstein, *Classical Mechanics*, Addison Wesley, 1980.

[11] Goldstein, *History of the Calculus of Variations*, Springer Verlag, 1980

[12] E. van Groesen & E.M. de Jager, *Mathematical structures in continuous dynamical systems*, North-Holland, Amsterdam, 1994.

[13] M.R. Hestenes, *Optimization theory, The finite dimensional case*, Wiley-Interscience, 1975.

[14] Ioffe & V.M. Tikhomirov, *Theory of Extremal problems*, North-Holland, 1979

[15] C. Lanczos, *The variational principles of mechanics*, Univ. Toronto Press, 1970.

[16] P. Lax, Integrals of nonlinear equations of evolution and solitary waves, *Comm. Pure Appl. Math.* **21**(1968)467-490

[17] V.M. Tikhomirov, *Stories about Maxima and Minima*, American Mathematical Society, 1990.

[18] J.L. Troutman, *Variational calculus with elementary convexity*, Springer, 1983.

[19] E. Zeidler, *Nonlinear functional analysis and its applications*, part III, Variational methods and optimization, Springer, 1985.