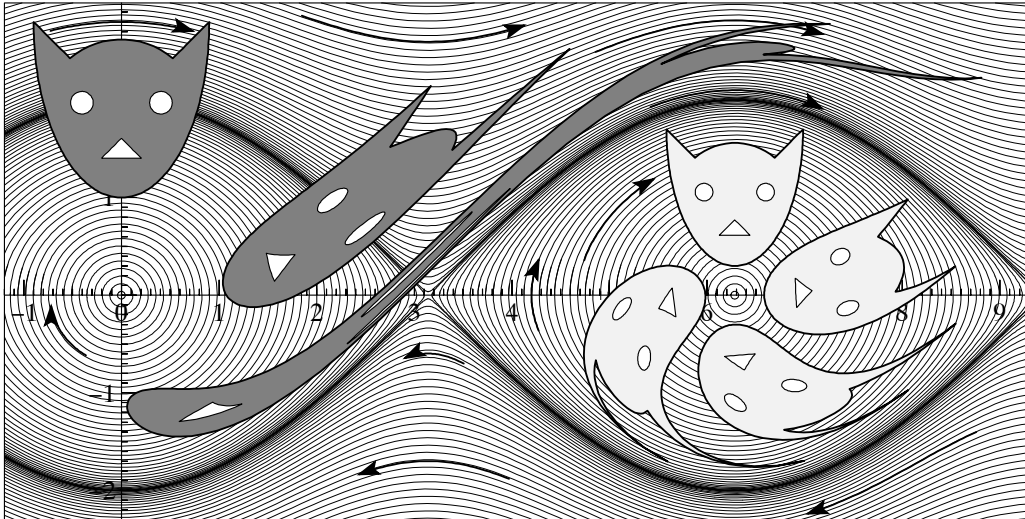


Geometric Numerical Integration of Ordinary Differential Equations



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1 Introduction

The field of structure-preserving or geometric discretisation [16, 31, 48, 10] has become a flourishing discipline of numerical analysis and scientific computing. Whereas most standard techniques put emphasis on the minimisation of local errors, for geometric numerical integrators the focus is rather on the preservation of global properties of the system. Therefore, what we call geometric structures are global properties, which can be defined independently of particular coordinate representations of the differential equations [16], e.g., topology, conservation laws, symmetries, constraints or identities. The preservation of geometric properties is advantageous for stability and crucial for long time simulations as it bounds global error growth and reduces numerical artefacts. Nowadays many families of geometric integrators are known, e.g., symplectic integrators, variational integrators, volume and integral preserving integrators.

1.1 Some Examples

In the following, we consider several examples, integrated with the following methods:

- explicit Euler:

$$\begin{aligned} q_{n+1} &= q_n + h H_p(q_n, p_n), \\ p_{n+1} &= p_n - h H_q(q_n, p_n), \end{aligned}$$

- implicit Euler:

$$\begin{aligned} q_{n+1} &= q_n + h H_p(q_{n+1}, p_{n+1}), \\ p_{n+1} &= p_n - h H_q(q_{n+1}, p_{n+1}), \end{aligned}$$

- symplectic Euler-A:

$$\begin{aligned} q_{n+1} &= q_n + h H_p(q_{n+1}, p_n), \\ p_{n+1} &= p_n - h H_q(q_{n+1}, p_n), \end{aligned}$$

- symplectic Euler-B:

$$\begin{aligned} p_{n+1} &= p_n - h H_q(q_n, p_{n+1}), \\ q_{n+1} &= q_n + h H_p(q_n, p_{n+1}). \end{aligned}$$

1.1.1 The Pendulum

The mathematical pendulum is a simple yet interesting system with quite a rich structure, which can be used to demonstrate many ideas in physics and numerics. For simplicity, we set the mass

$m = 1$, the rod is of length $l = 1$ and assumed to be massless, and the gravitational acceleration is set to $g = 1$. The system has one degree of freedom and its Hamiltonian is given by

$$H(q, p) = \frac{1}{2}p^2 - \cos q, \quad (1.1)$$

so that the equations of motion become

$$\dot{q} = \frac{\partial H}{\partial p} = p, \quad (1.2)$$

$$\dot{p} = -\frac{\partial H}{\partial q} = -\sin q. \quad (1.3)$$

As the system has just one degree of freedom, its solutions can be visualised in a phase diagram. In figure 1.1 we plot the contour lines of the Hamiltonian. As the energy H is conserved, the

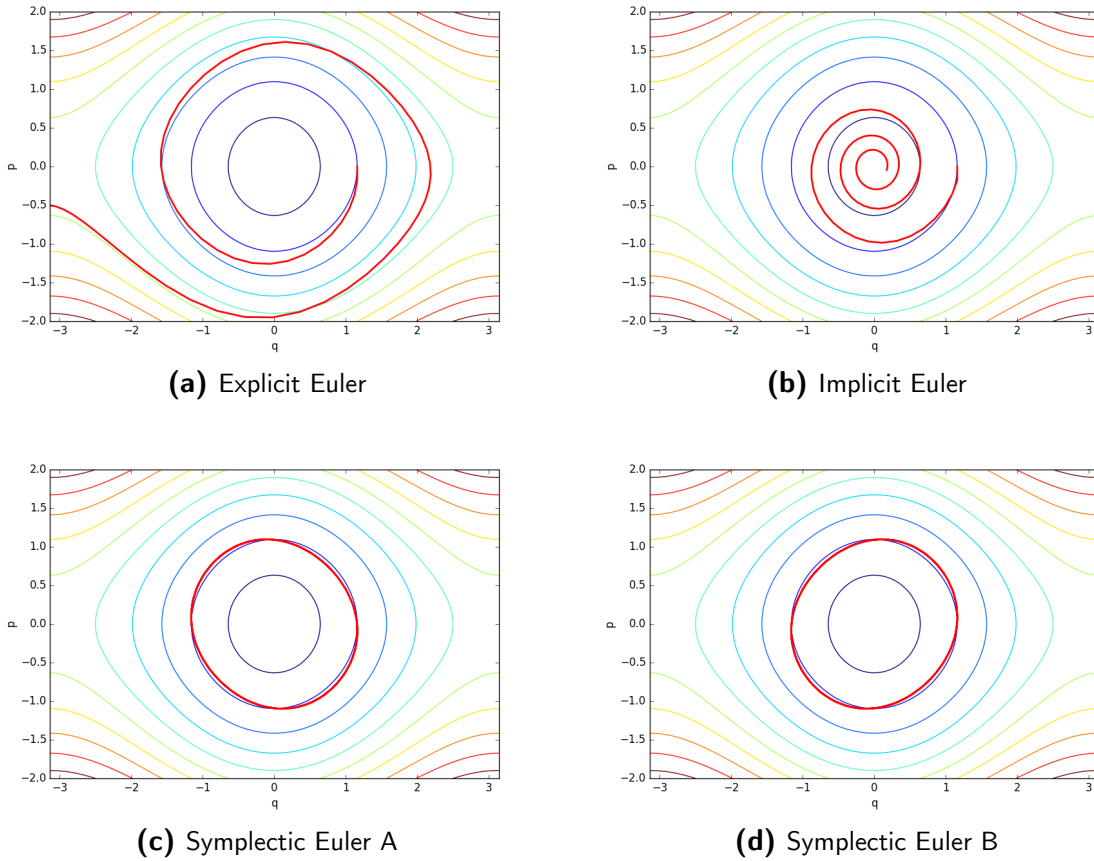


Fig. 1.1: Contour lines of the Hamiltonian for the pendulum and numerical solutions of various algorithms.

solutions follow those contour lines. This allows for a simple verification of numerical solutions of the equations of motion. Let us compare some standard methods, namely explicit Euler, implicit Euler and symplectic Euler. As initial values we use $(q_0, p_0) = (\arccos(0.4), 0.0)$ and a step size of $h_t = 0.2$.

We see that with the explicit Euler method, the system's energy is increasing until the system changes from a trapped orbit to a passing orbit, i.e., the topology of the orbit is not preserved. With the implicit Euler method, we observe the opposite. The method is dissipative, therefore the energy is decreasing, practically until the motion of the system comes to a halt. The symplectic

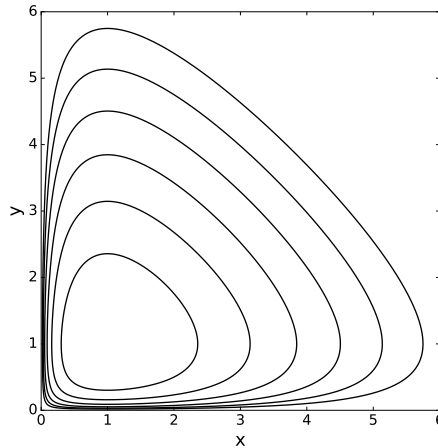
Euler methods, even though not following the orbit exactly, preserve the topology of the orbit for very long times and do neither loose nor gain energy. Of the three integrators, the symplectic Euler method is the only one which respects basic features of the system (approximate conservation of energy and the topology of the orbit), despite its relative large error at large time steps, which is due to the first-order nature of the scheme.

1.1.2 The Lotka-Volterra Model

Lotka-Volterra models are used in many fields, for example to describe population dynamics. We consider here a simple example with two species, predator and prey. Denote by x the prey population (say, rabbits) and by y the predator population (say, foxes). The equations describing the evolution of the two populations are given by

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} \alpha_1 x - \beta_1 xy \\ -\alpha_2 y + \beta_2 xy \end{pmatrix}, \quad (1.4)$$

with constants $\alpha_1, \alpha_2, \beta_1, \beta_2$. It turns out, that these equations form a noncanonical Hamiltonian system with two degrees of freedom. That is, the solution stays on contour lines of the Hamiltonian,



Equations (1.4) can also be written as

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = P(x, y) \nabla I(x, y) \quad (1.5)$$

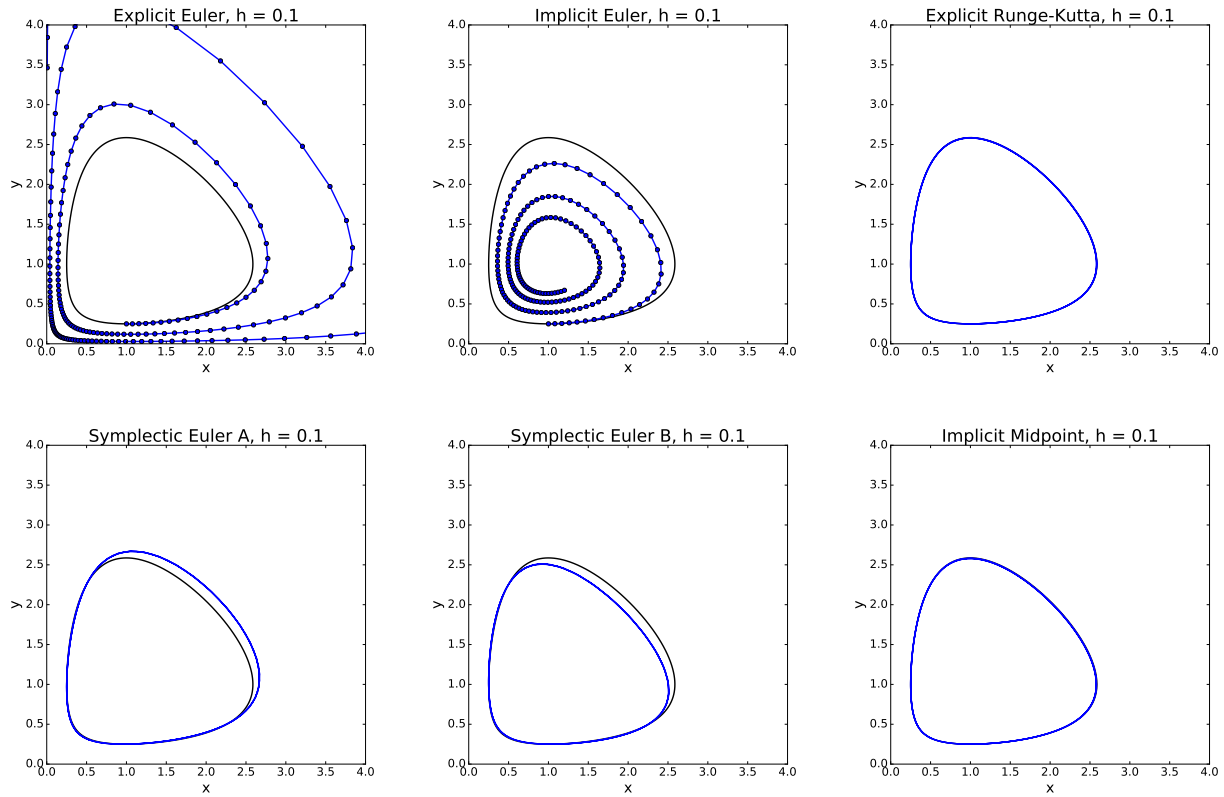
with Hamiltonian I ,

$$I(x, y) = \beta_2 x - \alpha_2 \log(x) + \beta_1 y - \alpha_1 \log(y), \quad (1.6)$$

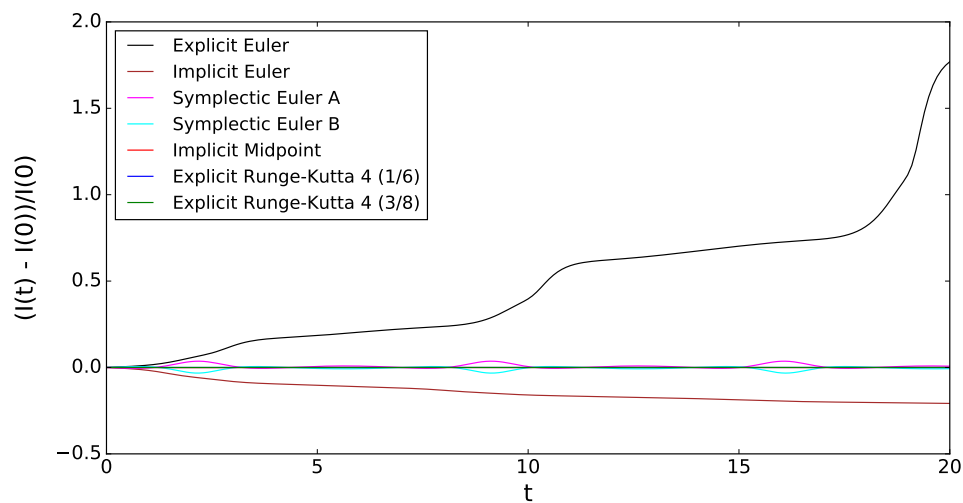
and noncanonical cosymplectic matrix P ,

$$P(x, y) = \begin{pmatrix} 0 & -xy \\ xy & 0 \end{pmatrix}. \quad (1.7)$$

Simulating this system for 200 time steps, we find the following behaviour with the various methods,

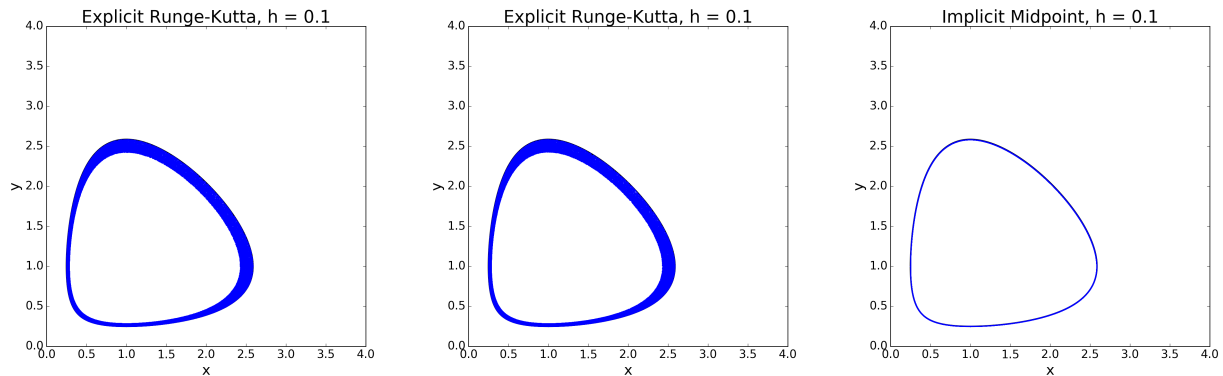


The error in the Hamiltonian of the various methods is as follows

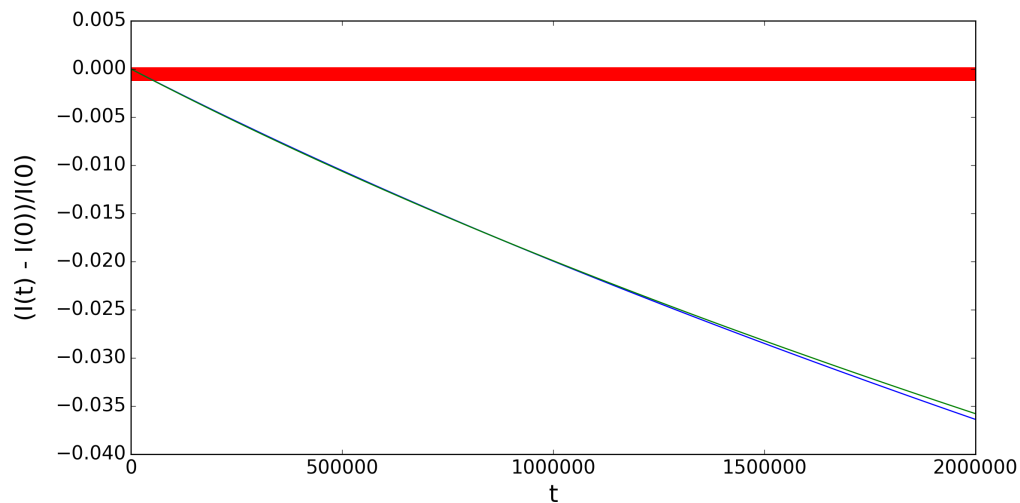


The explicit Euler method shows a severe increase in energy, while the implicit Euler method is strongly dissipative. All other methods stay close to the initial energy.

Running the simulation for much longer, namely for 20 million time steps, we observe the following behaviour,



with the corresponding errors in the Hamiltonian,



where we observe a clear drift in the simulations with the explicit Runge-Kutta methods (blue and green), while the error of the midpoint method (red) is bounded for very long times. Even though the error of the midpoint method initially is larger than that of the Runge-Kutta methods, the fact that it is just oscillating about the initial value but does not admit a drift, leads to a better long-time performance.

2 Some Numerical Analysis Background

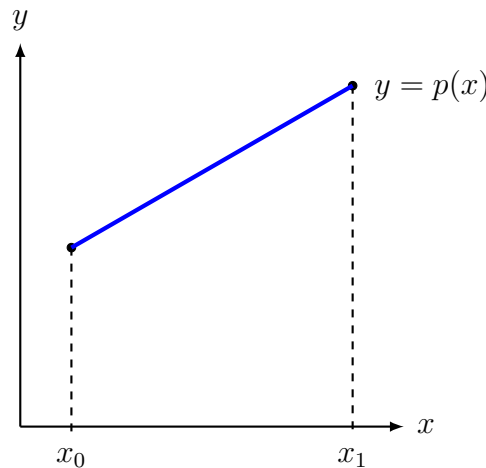
In this chapter we want to review some basic concepts from numerical analysis, which are needed to understand and design numerical integrators for ordinary differential equations, namely interpolation, approximation of function spaces and numerical quadrature. We will also review some standard methods for the numerical solution of ODEs. For more details on these topics see e.g. Quarteroni, Sacco, and Saleri [68, chapters 8-10].

2.1 Piecewise Polynomial Approximation

Piecewise polynomials are a type of functions, which can be used to approximate other more general functions, and which are easy to implement in computer codes. Typical applications include the fitting of data points in order to obtain predictions in regions where no data is available or to estimate the rate of change, or the approximation of complicated functions which are costly to evaluate by simpler functions. Moreover, the derivative and indefinite integral of a polynomial are easy to determine and are themselves polynomials. Therefore polynomials are often used in the design of numerical algorithms for approximating continuous functions like the unknown of some ordinary or partial differential equation.

2.1.1 Piecewise Linear Interpolation

Assume you are given two data points x_0, y_0 and x_1, y_1 which describe some unknown function and you are asked to provide the value of that function for some $x \in [x_0, x_1]$.



All you can do, is draw a straight line between the two points and find the y coordinate on that line corresponding to x . This is linear interpolation. The equation of the line connecting (x_0, y_0) and (x_1, y_1) is given by

$$p(x) = \frac{x_1 - x}{x_1 - x_0} y_0 + \frac{x - x_0}{x_1 - x_0} y_1, \quad x \in [x_0, x_1]. \quad (2.1)$$

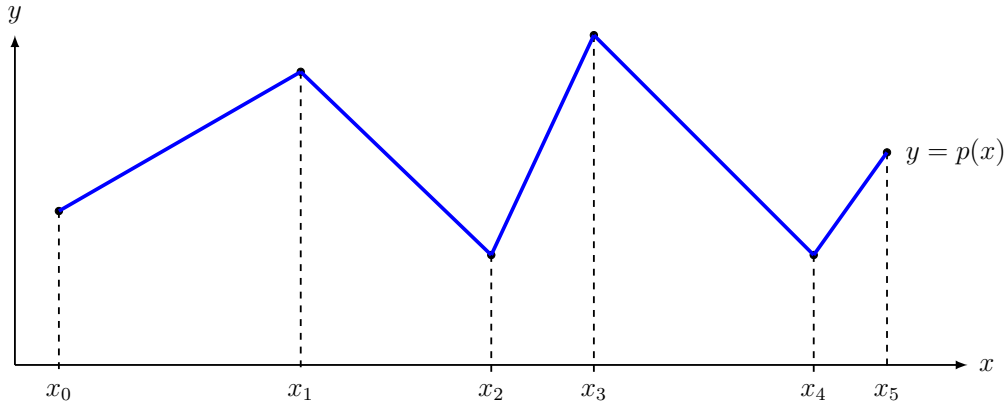


Fig. 2.1: Piecewise Linear Interpolation.

If we are given data at more than one point, that is values $y_0, y_1, y_2, \dots, y_n$ at points $x_0, x_1, x_2, \dots, x_n$, we can draw a line between each adjacent pair of points (see Figure 2.1). This corresponds to defining a piecewise function as follows,

$$p(x) = \begin{cases} y_0 \frac{x - x_0}{x_1 - x_0} + y_1 \frac{x_1 - x}{x_1 - x_0}, & x \in [x_0, x_1], \\ y_1 \frac{x_2 - x_1}{x_2 - x_1} + y_2 \frac{x_2 - x}{x_2 - x_1}, & x \in [x_1, x_2], \\ y_2 \frac{x_3 - x_2}{x_3 - x_2} + y_3 \frac{x_3 - x}{x_3 - x_2}, & x \in [x_2, x_3], \\ \dots & \dots \end{cases} \quad (2.2)$$

This is piecewise linear interpolation. It provides us with function estimates in the whole interval $[x_0, x_n]$. However, often this piecewise linear polynomial is not very accurate. In most cases, the function corresponding to the data will not have such sharp turns as in Figure 2.1 but a somewhat smoother behaviour. Moreover, such a piecewise linear approximation of the sought for function allows us only to compute first derivatives, which will be constant within each interval, so that all higher derivatives will vanish. On the interpolation points, not even first derivatives are defined.

2.1.2 Polynomial Interpolation

Instead of using linear polynomials for interpolating between two points, we could also use higher-order polynomials for interpolation within an interval containing several data points. This leads us to the problem of Lagrange interpolation, given below.

One of the most useful and well-known family of polynomials is the algebraic polynomials. These are functions of the form

$$p_n(x) = a_0 + a_1x + a_2x^2 + \dots + a_{n-1}x^{n-1} + a_nx^n, \quad (2.3)$$

mapping the set of real numbers into itself, where n is a non-negative integer and a_0, \dots, a_n are real constants.

Definition 2.1 (Lagrange Interpolation). *Given finitely many distinct real numbers x_0, x_1, \dots, x_n , referred to as nodes, and for each x_i a corresponding value y_i , the problem of Lagrange interpolation is to find a polynomial function $p(x)$ of degree at most n , such that*

$$p(x_i) = y_i, \quad i = 0, \dots, n. \quad (2.4)$$

This problem has a unique solution. Write the sought after polynomial in the form (2.3), as a sum of monomials, with the coefficients a_i to be determined. This leads to a system of $n + 1$ linear equations in $n + 1$ unknowns,

$$Xa = y, \quad (2.5)$$

with

$$X = \begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{pmatrix}, \quad a = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix}, \quad y = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{pmatrix}. \quad (2.6)$$

The $(n+1) \times (n+1)$ matrix X on the left-hand side is called a Vandermonde matrix. The question of existence and uniqueness of the interpolating polynomial boils down to whether this matrix is invertible. By recursion on n one can show that the determinant of X is given by

$$\det X = \prod_{0 \leq j < i \leq n} (x_i - x_j), \quad (2.7)$$

which implies that X is non-singular whenever all x_i are distinct, so that the linear system (2.6) always has a unique solution.

2.1.3 Weierstrass Approximation Theorem

The algebraic polynomials, introduced in the previous section, have the particularly useful property of uniformly approximating the continuous functions. That means for any given function, defined and continuous on a closed and bounded interval, there exists a polynomial that is as close to the given function as desired (see Figure 2.2). This is made precise in the Weierstrass approximation theorem.

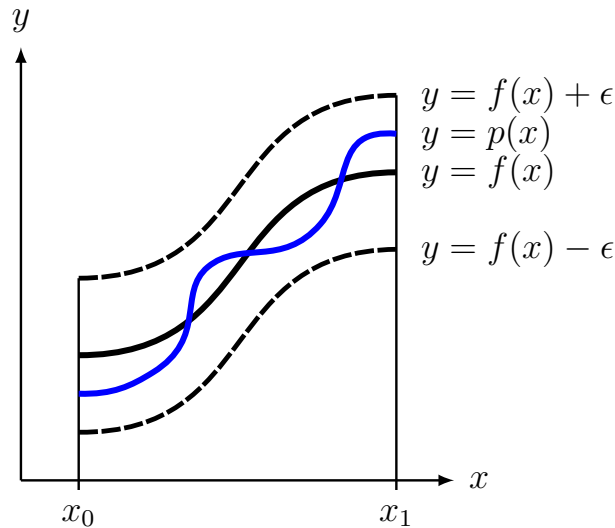


Fig. 2.2: Weierstrass Approximation Theorem.

Theorem 2.2. *Weierstrass Approximation Theorem.* Suppose that f is a function defined and continuous on the interval $[x_0, x_1]$. For each $\epsilon > 0$, there exists a polynomial $p(x)$, with the property that

$$|f(x) - p(x)| < \epsilon, \quad \text{for all } x \in [x_0, x_1]. \quad (2.8)$$

Proof. The proof of this theorem can be found in most textbooks on real analysis. \square

2.1.4 Spaces of Polynomials

Let $I = [x_0, x_1]$ be an interval on the real axis and let $\mathbb{P}_1(I)$ denote the vector space of linear functions on I , defined by

$$\mathbb{P}_1(I) = \{p : p(x) = a_0 + a_1x, x \in I, a_0, a_1 \in \mathbb{R}\}. \quad (2.9)$$

That is $\mathbb{P}_1(I)$ contains all functions of the form $p(x) = a_0 + a_1x$ on I .

A natural basis for $\mathbb{P}_1(I)$ is the monomial basis $\{1, x\}$, since any function $p(x)$ in $\mathbb{P}_1(I)$ can be written as a linear combination of 1 and x , that is a constant a_0 times 1 plus another constant a_1 times x . Thereby p is uniquely determined by specifying a_0 and a_1 , the coefficients of the linear combination. We say that p has two degrees of freedom, a_0 and a_1 .

However, a_0 and a_1 are not the only degrees of freedom possible for p . To see this, recall that a line, or a linear function, is uniquely determined by requiring it to pass through any two given points. Obviously, there are many pairs of points that can specify the same line. In fact, any two points within the interval I will do as degree of freedoms for p . In particular, p can be uniquely determined by its values $y_0 = p(x_0)$ and $y_1 = p(x_1)$ at the endpoints x_0 and x_1 of I . To see this, we just have to insert these values into (2.6), giving

$$\begin{pmatrix} 1 & x_0 \\ 1 & x_1 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \end{pmatrix}, \quad (2.10)$$

and solve this linear system. This provides us with a general algorithm to compute and evaluate the interpolating polynomial:

1. form the Vandermonde matrix (2.6),
2. solve the linear system (2.5),
3. evaluate the polynomial (2.3).

This approach, however, is not very efficient. Instead, knowing that we can completely specify any function in $\mathbb{P}_1(I)$ by its node values y_0 and y_1 , we can introduce a new basis $\{l^{1,1}, l^{1,2}\}$ for $\mathbb{P}_1(I)$. This basis is called a nodal basis and is defined by

$$l^{1,j}(x_i) = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases} \quad i, j = 0, 1. \quad (2.11)$$

From this definition we see that each basis function $l^{1,j}$, $j = 0, 1$, is a linear function, which takes on the value 1 at node x_j and 0 at the other node. The basis functions take the following explicit form on I ,

$$l^{1,0}(x) = \frac{x - x_1}{x_0 - x_1}, \quad l^{1,1}(x) = \frac{x - x_0}{x_1 - x_0}. \quad (2.12)$$

This follows from the definition (2.11) or by solving the linear system (2.10) with $(1, 0)^T$ and $(0, 1)^T$ as right-hand sides.

The nodal basis (2.11) allows us to express any function p in $\mathbb{P}_1(I)$ as a linear combination of $l^{1,0}$ and $l^{1,1}$ with y_0 and y_1 as coefficients,

$$p(x) = y_0 l^{1,0}(x) + y_1 l^{1,1}(x). \quad (2.13)$$

This is in contrast to the monomial basis, which given the node values requires inversion of the Vandermonde matrix to determine the corresponding coefficients a_0 and a_1 .

2.1.5 Lagrange Polynomials

Equations (2.1) and (2.13), which are equivalent, define the linear Lagrange interpolating polynomial through (x_0, y_0) and (x_1, y_1) ,

$$p(x) = y_0 l^{1,0}(x) + y_1 l^{1,1}(x) = y_0 \frac{x - x_1}{x_0 - x_1} + y_1 \frac{x - x_0}{x_1 - x_0}. \quad (2.14)$$

The construction that lead to this polynomial can be generalised to polynomials of arbitrary degree n that pass through the $n + 1$ points

$$(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n).$$

If we define the corresponding Lagrange polynomials of degree n by

$$l^{n,j}(x) = \frac{(x - x_0)(x - x_1) \cdots (x - x_{j-1})(x - x_{j+1}) \cdots (x - x_n)}{(x_j - x_0)(x_j - x_1) \cdots (x_j - x_{j-1})(x_j - x_{j+1}) \cdots (x_j - x_n)} = \prod_{\substack{i=0 \\ i \neq j}}^n \frac{x - x_i}{x_j - x_i}, \quad (2.15)$$

then

$$l^{n,j}(x_i) = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases} \quad i, j = 0, 1, \dots, n, \quad (2.16)$$

so that

$$p(x) = \sum_{j=0}^n y_j l^{n,j}(x) \quad (2.17)$$

solves the Lagrange interpolation problem. This formula is known as *Lagrange's form* of the interpolating polynomial. The polynomial it determines is the same as that determined by solving the Vandermonde system but there is no need to solve a linear system to compute it.

2.1.6 Interpolation Error

Suppose that there is a function f , probably not a polynomial, defined on an interval containing all the nodes and such that the values are just the values of $y_i = f(x_i)$. Consider the difference

$$E(x) = f(x) - p(x). \quad (2.18)$$

To get a handle on this error, fix one point x and consider the function

$$G(t) = [f(x) - p(x)](t - x_0) \cdots (t - x_n) - [f(t) - p(t)](x - x_0) \cdots (x - x_n). \quad (2.19)$$

This function G vanishes when t is one of the $n + 1$ nodes x_j . It is also constructed so that $G(t) = 0$ when $t = x$. Thus the function G has $n + 2$ roots. We shall suppose that the function f is differentiable as many times as needed. Applying Rolle's theorem or the Mean Value Theorem, we conclude that the derivative G' has at least $n + 1$ roots. The same reasoning shows that G'' has n roots and, finally, that $G^{(n+1)}(\xi) = 0$ for some ξ in the smallest interval containing the x_j and x . We have that

$$p^{(n+1)}(\xi) = 0,$$

as well as

$$\frac{d^{n+1}}{dx^{n+1}}[(t-x_0)\cdots(t-x_n)] = (n+1)!,$$

so that

$$f(x) - p(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi) (x-x_0)\cdots(x-x_n). \quad (2.20)$$

This leads us to the following theorem.

Theorem 2.3 (Error Formula for Lagrange Interpolation). *Suppose $f \in C^{n+1}(I)$ on some interval I contain $n+1$ distinct nodes and another point x . Let p be the Lagrange interpolating polynomial interpolating the values $f(x_i)$ at x_i . Then, for any point there is a number ξ in the least interval containing the x_i and x , such that (2.20) holds.*

It is not easy to get a good quantitative bound on the error from this formula, even for quite simple functions $f(x)$ and simple point sets x_i . This is because, the higher derivatives $f^{(n+1)}$ generally become very complicated. But we can learn a lot by studying the final factor,

$$\omega(x) = (x-x_0)\cdots(x-x_n), \quad (2.21)$$

often called the error product associated to the nodes.

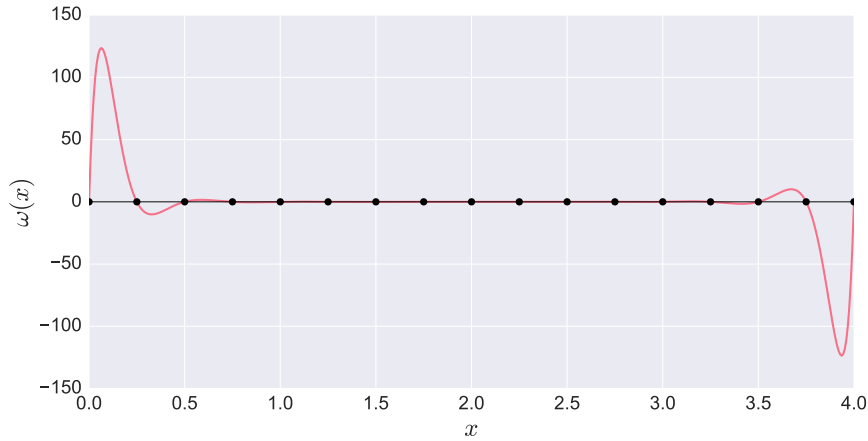


Fig. 2.3: The error product for 17 equally spaced abscissa from 0 to 4.

The error product highlights a big problem with Lagrange interpolation using equally spaced nodes as illustrated in Figure 2.3, showing the error product for 17 equally spaced abscissas from 0 to 4. Near the ends of the interval the error is many orders of magnitude larger than near the centre. This is a major reason why Lagrange interpolation is rarely used for large number of points (about 10 or more). For larger n it tends to have large errors near the interval end points. In particular, if we fix the interval and the function, say a very nice smooth function, and add more and more equally spaced points to obtain Lagrange interpolating polynomials of higher and higher degree, then it is usually not the case that the resulting polynomials converge to the function. To the contrary, the polynomials often oscillate wildly near the interval ends. A famous example, due to Runge, is $f(x) = 1/(1+x^2)$ on $[-5, +5]$, shown in Figure 2.4 for $n = 12$.

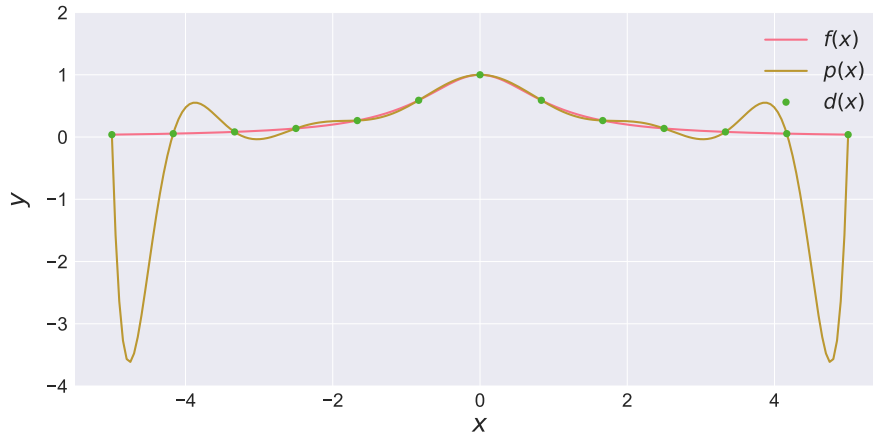


Fig. 2.4: Runge's example with 13 points and equidistant nodes.

2.1.7 Chebyshev and Legendre Nodes

A question that remains is how to choose the nodes for the Lagrange polynomial. If we interpolate data, they are prescribed by the data points, but if we interpolate a function $f(x)$, we are free to choose the nodes.

We discussed that for equidistant nodes the Lagrange interpolating polynomials do not approximate well as the number of points is increased. A way around this is to use Lagrange interpolation with a better choice of points. One such family of points is provided by Chebyshev nodes, another one by Legendre nodes. These are the roots of the Chebyshev and Legendre polynomials, $T(x)$ and $P(x)$, respectively, given by the recursion formulas

$$T_{n+1}(x) = 2x T_n(x) - T_{n-1}(x), \quad T_0 = 1, \quad (2.22)$$

and

$$P_{n+1}(x) = \frac{2n+1}{n+1} x P_n(x) - \frac{n}{n+1} P_{n-1}(x), \quad P_0 = 1. \quad (2.23)$$

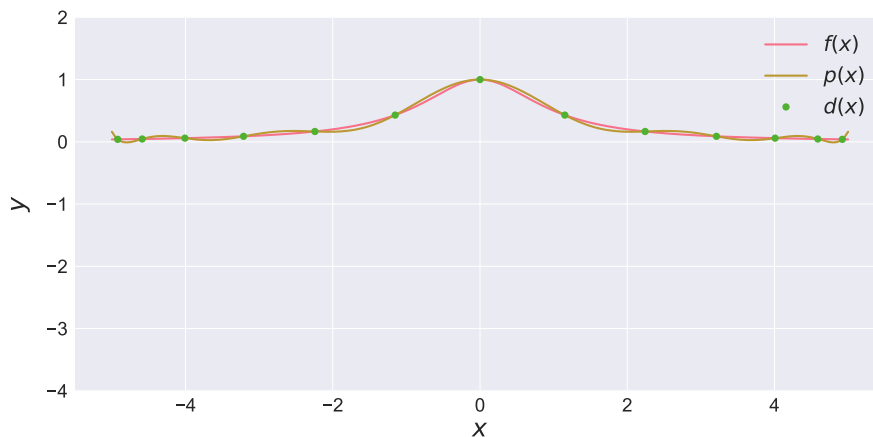


Fig. 2.5: Runge's example with 13 points and Legendre nodes.

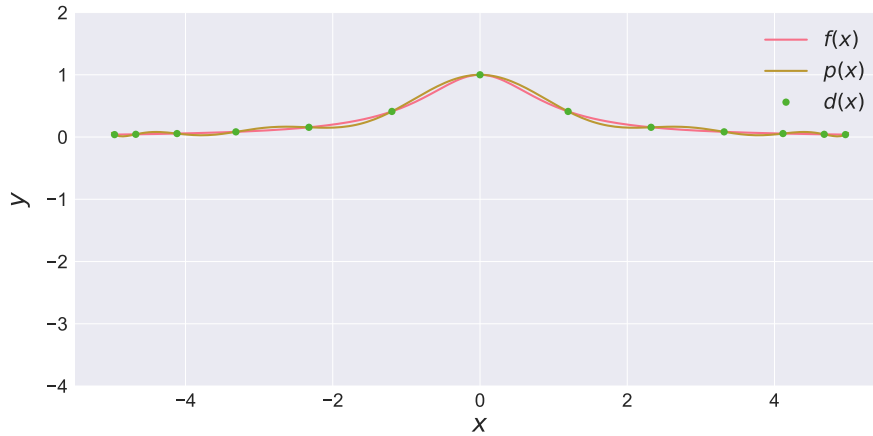


Fig. 2.6: Runge's example with 13 points and Chebyshev.

2.1.8 Spaces of Piecewise Polynomials

In order to interpolate between values given at a set of distinct points on an interval, we have seen how to either compute the corresponding Lagrange interpolating polynomial as well as how to use piecewise linear interpolation. We know, e.g., from Runge's example, that for more than a few points, the Lagrange interpolating polynomial may be highly oscillatory even when the values are taken from a smooth underlying function. Moreover, it is clear, that a piecewise linear approximation often is not very accurate. An alternative is to combine both approaches and use piecewise polynomials instead, which give good approximations to smooth functions. Unlike polynomials, they are not infinitely differentiable functions. However we can choose the degree of smoothness (C^0 , C^1 , ...) according to our needs, even though we will restrict to C^0 for the moment.

The basic idea is to subdivide the domain into smaller subintervals, where on each subinterval the interpolating function p is given by a polynomial. Let $I = [0, L]$ be an interval and let the $n + 1$ nodes $\{x_i\}_{i=0}^n$ define a partition

$$\mathcal{I} : 0 = x_0 < x_1 < x_2 < \cdots < x_{n-1} < x_n = L \quad (2.24)$$

of I into n subintervals $I_i = [x_{i-1}, x_i]$, $i = 1, 2, \dots, n$, of length $h_i = x_i - x_{i-1}$. The partition \mathcal{I} is often referred to as a mesh. On the mesh \mathcal{I} we define the space V_h of continuous piecewise functions by

$$V_h = \{p : p \in C^0(I), p|_{I_i} \in \mathbb{P}_n(I_i)\}, \quad (2.25)$$

where $C^0(I)$ denotes the space of continuous functions on I and $\mathbb{P}_n(I_i)$ denotes the space of polynomials of degree n on I_i . A basis for V_h can be constructed by defining Lagrange polynomials of degree n in each subinterval I_i . In order to do so, we need to specify $n + 1$ internal nodes $X_{i,j}$, $0 \leq j \leq n$, in each interval I_i , which can for example be chosen as equidistant nodes (with the discussed disadvantages), Chebyshev nodes or Legendre nodes. In this context the nodes x_i are often referred to as *external nodes* or *macro-nodes* while the $X_{i,j}$ are referred to as *internal nodes* or *micro-nodes*. If one degree of freedom is placed at the start- and one at the end-point of each subinterval, respectively, continuity of p between adjacent subintervals is automatically enforced.

2.2 Numerical Quadrature

The need for numerical quadrature often arises for evaluating the definite integral of a function that has no explicit antiderivative (indefinite integral) or whose antiderivative is not easy to obtain. The idea of numerical quadrature is to approximate $\int_a^b f(x) dx$ by a sum $\sum_{i=0}^n b_i f(x_i)$.

2.2.1 Quadrature Formulas

Many methods of quadrature are based on the interpolation polynomials introduced in the previous section. The basic idea is to select a set of distinct nodes $\{x_0, \dots, x_n\}$ from the interval $[a, b]$ and integrate the Lagrange interpolating polynomial

$$p_n(x) = \sum_{i=0}^n f(x_i) l^{n,i}(x) \quad (2.26)$$

over $[a, b]$ to obtain

$$\int_a^b f(x) dx \approx \int_a^b \sum_{i=0}^n f(x_i) l^{n,i}(x) dx \approx \sum_{i=0}^n b_i f(x_i), \quad (2.27)$$

where

$$b_i = \int_a^b l^{n,i}(x) dx, \quad \text{for each } i = 0, 1, \dots, n. \quad (2.28)$$

Such formulas are called *interpolatory quadrature rules*. Some well known and widely used quadrature formulas are obtained by using first and second Lagrange polynomials with equidistant nodes.

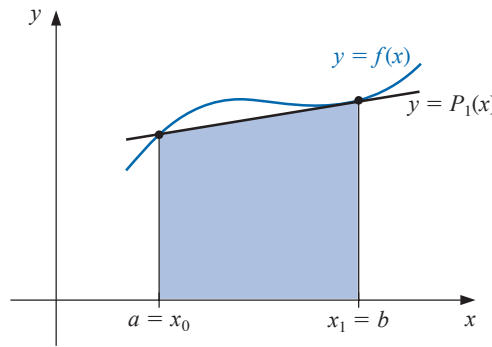


Fig. 2.7: Trapezoidal rule.

Trapezoidal Rule To derive the trapezoidal rule, let $x_0 = a$ and $x_1 = b$ and use the linear Lagrange polynomial

$$p_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1).$$

Then

$$\int_a^b f(x) dx \approx \int_{x_0}^{x_1} \left[\frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) \right] dx = \frac{h}{2} [f(x_0) + f(x_1)], \quad (2.29)$$

with $h = b - a$.

Midpoint Rule To derive the trapezoidal rule, let $x_0 = (a + b)/2$ and use the constant Lagrange polynomial

$$p_0(x) = f(x_0),$$

so that

$$\int_a^b f(x) dx \approx \int_{x_0-h}^{x_0+h} f(x_0) dx = 2h f(x_0), \quad (2.30)$$

with $h = (b - a)/2$.

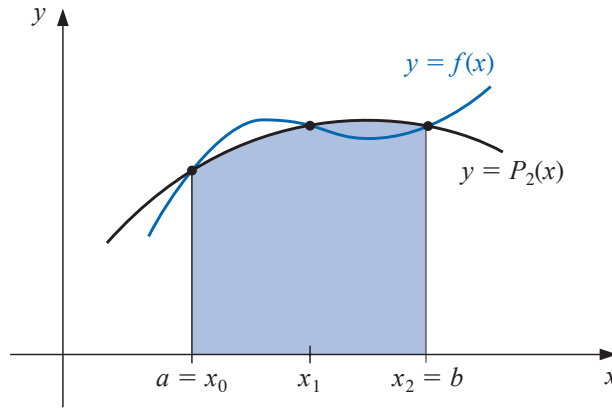


Fig. 2.8: Simpson rule.

Simpson Rule Simpson's rule results from integrating over $[a, b]$ the second Lagrange polynomial with equally-spaced nodes $x_0 = a$, $x_1 = a + h/2$, $x_2 = b$, where $h = b - a$,

$$p_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2),$$

so that

$$\begin{aligned} \int_a^b f(x) dx \approx \int_{x_0}^{x_1} \sum_{i=0}^n \left[\frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) \right. \\ \left. + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2) \right] dx = \frac{h}{6} [f(x_0) + 4f(x_1) + f(x_2)]. \end{aligned} \quad (2.31)$$

2.2.2 Newton-Cotes Formulas

The Trapezoidal, Simpson and midpoint rules are examples of a class of methods known as Newton-Cotes formulas. There are two types of Newton-Cotes formulas, open and closed.

Closed Newton-Cotes Formulas The $(n + 1)$ point closed Newton-Cotes formula uses nodes $x_i = x_0 + ih$ for $i = 0, 1, \dots, n$, where $x_0 = a$, $x_n = b$ and $h = (b - a)/n$ (see Figure 2.9). It is called closed because the endpoints of the closed interval $[a, b]$ are included as nodes.

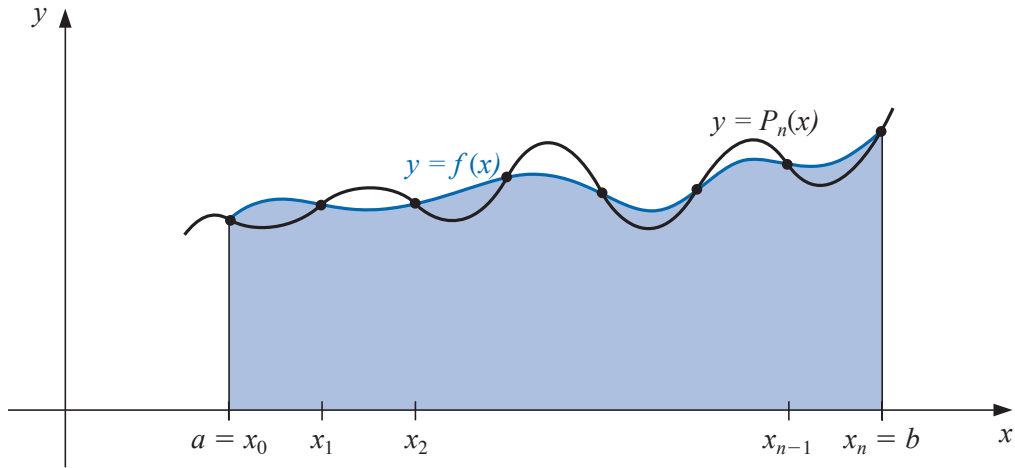


Fig. 2.9: Closed Newton-Cotes Formulas.

The formula assumes the form

$$\int_a^b f(x) dx \approx \sum_{i=0}^n b_i f(x_i), \quad (2.32)$$

where

$$b_i = \int_{x_0}^{x_n} l^{n,i}(x) dx = \int_{x_0}^{x_n} \prod_{\substack{i=0 \\ i \neq j}}^n \frac{x - x_i}{x_j - x_i} dx. \quad (2.33)$$

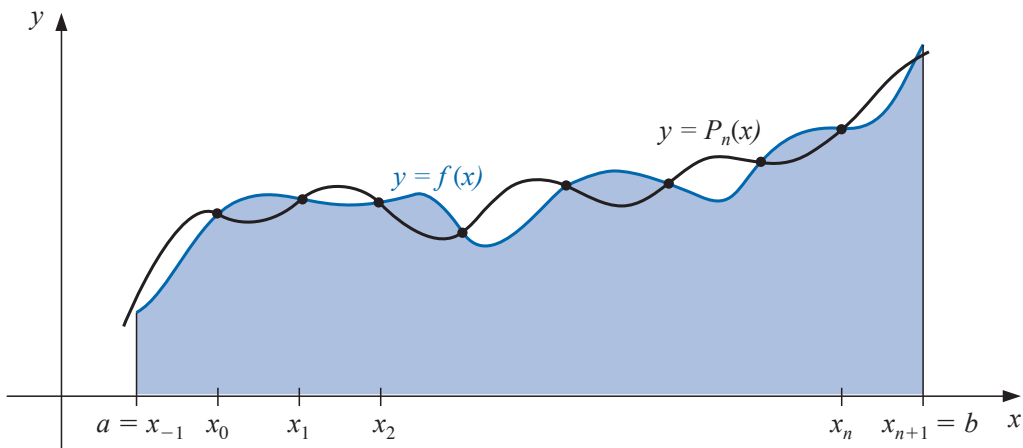


Fig. 2.10: Open Newton-Cotes Formulas.

Open Newton-Cotes Formulas The open Newton-Cotes formulas do not include the endpoints of $[a, b]$ as nodes. They use the nodes $x_i = x_0 + ih$, $i = 0, 1, \dots, n$, where $h = (b-a)/(n+2)$, $x_0 = a+h$ and $x_n = b-h$. We label the endpoints by setting $x_{-1} = a$ and $x_{n+1} = b$, as shown in Figure 2.10. Open formulas contain all the nodes used for the approximation within the open interval (a, b) .

The formulas become

$$\int_a^b f(x) dx \approx \sum_{i=0}^n b_i f(x_i), \quad (2.34)$$

where

$$b_i = \int_{x_{-1}}^{x_{n+1}} l^{n,i}(x) dx = \int_{x_{-1}}^{x_{n+1}} \prod_{\substack{i=0 \\ i \neq j}}^n \frac{x - x_i}{x_j - x_i} dx. \quad (2.35)$$

The Newton-Cotes formulas are exact if f is a polynomial of degree at most n .

2.2.3 Composite Quadrature

The Newton-Cotes formulas are generally unsuitable for use over large integration intervals. This is due to the problems with respect to the stability of Lagrange polynomials with many equidistant nodes, discussed earlier. The Newton-Cotes formulas are based on interpolatory polynomials that use equally-spaced nodes, a procedure that is inaccurate over large intervals because of the oscillatory nature of high-degree polynomials. This problem can be remedied by a piecewise approach, where the integration interval $[a, b]$ is split into n subintervals and on each subinterval low-order Newton-Cotes formulas are used.

As an example consider the composite trapezoidal rule (see Figure 2.11), given by

$$\int_a^b f(x) dx \approx \frac{h}{2} \left[f(a) + 2 \sum_{j=0}^{n-1} f(x_j) + f(b) \right], \quad (2.36)$$

for $h = (b - a)/n$.

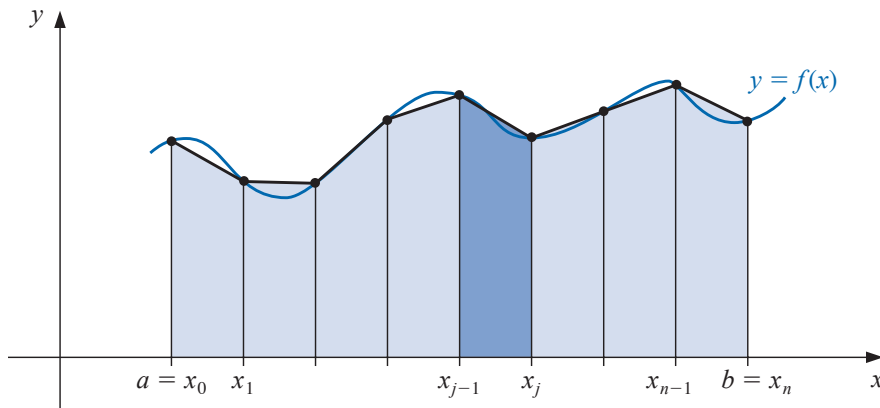


Fig. 2.11: Composite Trapezoidal Rule.

As another example consider the composite midpoint rule (see Figure 2.12), given by

$$\int_a^b f(x) dx \approx 2h \sum_{j=0}^{n/2} f(x_{2j}), \quad (2.37)$$

for $h = (b - a)/(n + 2)$ and n is assumed to be even.

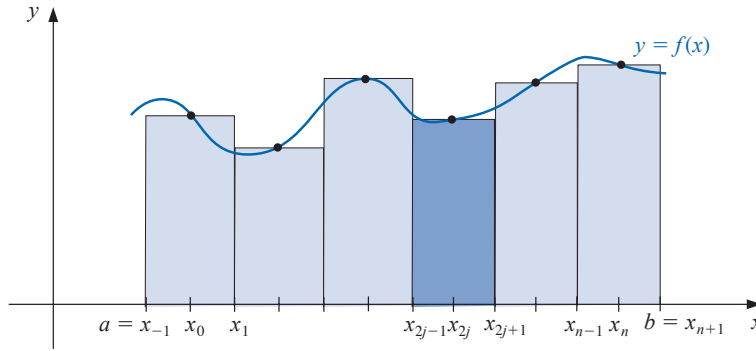


Fig. 2.12: Composite Midpoint Rule.

2.2.4 Gaussian Quadrature

In the derivation of the Newton-Cotes formulas we assumed that the nodes were equally spaced and fixed. This led to quadrature formulas which are exact if f is a polynomial of degree at most n . The main idea for obtaining more accurate quadrature formulas is to treat the nodes as additional degrees of freedom. Gaussian quadrature chooses the nodes for evaluation in an optimal, rather than equidistant, way. The nodes x_0, x_1, \dots, x_n in the interval $[a, b]$ and coefficients b_0, b_1, \dots, b_n , are chosen to minimise the expected error obtained in the approximation

$$\int_a^b f(x) dx \approx \sum_{i=0}^n b_i f(x_i). \quad (2.38)$$

The coefficients b_0, b_1, \dots, b_n in the approximation formula are arbitrary, and the nodes x_0, x_1, \dots, x_n are restricted only by the fact that they must lie in $[a, b]$, the interval of integration. This gives us $2n + 2$ parameters to choose. If the coefficients of a polynomial are considered parameters, the class of polynomials of degree at most $2n + 1$ also contains $2n + 2$ parameters. This, then, is the largest class of polynomials for which it is reasonable to expect a formula to be exact. With the proper choice of the values and constants, exactness on this set can be obtained.

To illustrate the procedure for choosing the appropriate parameters, we will show how to select the coefficients and nodes when $n = 1$ and the interval of integration is $[-1, +1]$. Suppose we want to determine b_0, b_1, x_0 , and x_1 so that the integration formula

$$\int_{-1}^{+1} f(x) dx \approx b_0 f(x_0) + b_1 f(x_1) \quad (2.39)$$

gives the exact result whenever $f(x)$ is a polynomial of degree $2(1) + 1 = 3$ or less, that is, when

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3, \quad (2.40)$$

for some collection of constants, a_0, a_1, a_2 , and a_3 . Because

$$\int (a_0 + a_1 x + a_2 x^2 + a_3 x^3) dx = a_0 \int 1 dx + a_1 \int x dx + a_2 \int x^2 dx + a_3 \int x^3 dx, \quad (2.41)$$

this is equivalent to showing that the formula gives exact results when $f(x)$ is 1, x , x^2 , and x^3 .

Hence we need b_0 , b_1 , x_0 , and x_1 , so that

$$b_0 \cdot 1 + b_1 \cdot 1 = \int_{-1}^{+1} 1 \, dx = 2, \quad b_0 \cdot x_0 + b_1 \cdot x_1 = \int_{-1}^{+1} x \, dx = 0, \quad (2.42)$$

$$b_0 \cdot x_0^2 + b_1 \cdot x_1^2 = \int_{-1}^{+1} x^2 \, dx = \frac{2}{3}, \quad b_0 \cdot x_0^3 + b_1 \cdot x_1^3 = \int_{-1}^{+1} x^3 \, dx = 0, \quad (2.43)$$

$$(2.44)$$

This system of equations has the unique solution

$$b_0 = 1, \quad b_1 = 2, \quad x_0 = -\frac{\sqrt{3}}{3}, \quad x_1 = +\frac{\sqrt{3}}{3}, \quad (2.45)$$

which gives the approximation formula

$$\int_{-1}^{+1} f(x) \, dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right). \quad (2.46)$$

This formula produces the exact result for every polynomial of degree 3 or less.

The technique we have described could be used to determine the nodes and coefficients for formulas that give exact results for higher-degree polynomials, but an alternative method obtains them more easily. The nodes x_0, x_1, \dots, x_n needed to produce an integral approximation formula that gives exact results for any polynomial of degree less than $2n+2$ are the roots of the Legendre polynomial of degree $n+1$.

2.3 Numerical Solution of ODEs

Ordinary differential equations are ubiquitous in science and engineering. Many can be solved analytically, but even more cannot. Numerical integration techniques provide an important tool for studying such equations. In the following, we will focus on *initial value problems* like the following,

$$\dot{x}(t) = f(x(t)), \quad x(t_0) = x_0, \quad (2.47)$$

with f a vector field $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$. The solution $x(t)$ is a curve $x : \mathcal{I} \rightarrow \mathbb{R}^d$ with $\mathcal{I} \subset \mathbb{R}$, which satisfies (2.47). If f is continuously differentiable, then there exists a unique solution at least locally on some open interval containing t_0 .

Consider for example the growth of a population of rabbits. Here, $x(t)$ denotes the number of rabbits at time t . The change of x (here, the growth of the population) is proportional to the current size of the population, that is

$$\dot{x}(t) = \alpha x(t), \quad x(t_0) = x_0, \quad \alpha > 0. \quad (2.48)$$

The explicit solution to this problem is exponential growth,

$$x(t) = x_0 e^{\alpha(t-t_0)}. \quad (2.49)$$

The behaviour becomes more complicated if we add a second species y of predators, say foxes. The growth of the rabbit population is still proportional to its current size, but it is also inversely

proportional to the population size of the foxes. Similarly, the growth of the fox population is inversely proportional to its current size and proportional to the population of rabbits. The resulting (nonlinear) system of equations reads

$$\dot{x}(t) = \alpha_1 x(t) - \beta_1 y(t) x(t), \quad x(t_0) = x_0, \quad \alpha_1, \beta_1 > 0, \quad (2.50a)$$

$$\dot{y}(t) = -\alpha_2 y(t) + \beta_2 x(t) y(t), \quad y(t_0) = y_0, \quad \alpha_2, \beta_2 > 0. \quad (2.50b)$$

Diving the two equations, we find

$$\frac{\dot{x}(t)}{\dot{y}(t)} = \frac{x(t)(\alpha_1 - \beta_1 y(t))}{y(t)(\beta_2 x(t) - \alpha_2)}, \quad (2.51)$$

so that

$$\dot{x}(t) \frac{\beta_2 x(t) - \alpha_2}{x(t)} = \dot{y}(t) \frac{\alpha_1 - \beta_1 y(t)}{y(t)}, \quad (2.52)$$

or

$$0 = \dot{x}(t) \frac{\beta_2 x(t) - \alpha_2}{x(t)} - \dot{y}(t) \frac{\alpha_1 - \beta_1 y(t)}{y(t)} \equiv \frac{d}{dt} I(x, y), \quad (2.53)$$

with

$$I(x, y) = \beta_2 x - \alpha_2 \ln(x) + \alpha_1 y - \beta_1 \ln(y). \quad (2.54)$$

This means that I is constant along solutions (x, y) of (2.50). In other words, I is an *invariant* or a *first integral* of the system and solutions of (2.50) with $x > 0$ and $y > 0$ lie on level sets of I . This is very useful information when judging the quality of numerical solutions of (2.50).

2.3.1 Elementary One-Step Methods

Explicit Euler

Euler's method is the most elementary approximation technique for solving initial-value problems. The idea is to write down the first terms in the Taylor expansion of the solution $x(t)$ at t_0 and use the initial value and the differential equation at $t = t_0$,

$$x(t_0 + h) = x(t_0) + h\dot{x}(t_0) + \mathcal{O}(h^2) = x(t_0) + hf(t_0, x_0) + \mathcal{O}(h^2). \quad (2.55)$$

Choosing a small step size $h > 0$ and neglecting the higher-order terms in h , an approximation x_1 to $x(t_1)$ at time $t_1 = t_0 + h$ is obtained by

$$x_1 = x_0 + hf(t_0, x_0). \quad (2.56)$$

Then, use this value x_1 as starting value for a further step, which then yields an approximation to the solution at $t_2 = t_1 + h$ as $x_2 = x_1 + hf(t_1, x_1)$. Continuing in this way, after n steps we take $x_n = x(t_n)$ as the starting value for computing an approximation at $t_{n+1} = t_n + h$ as

$$x_{n+1} = x_n + hf(t_n, x_n). \quad (2.57)$$

The computational cost of the method lies in the evaluation of the function f . The quality of the approximation x_n depends on two aspects: the error made by truncating the Taylor expansion and the error introduced by continuing from approximate solution values. These two aspects are captured in the notions of *consistency* and *stability*, respectively, and are fundamental to all numerical methods for ordinary differential equations.

Implicit Euler

A minor looking change in the Euler method (2.57) makes a big difference: taking as argument of f the new value instead of the previous one yields,

$$x_{n+1} = x_n + hf(t_{n+1}, x_{n+1}), \quad (2.58)$$

from which x_{n+1} is now determined implicitly. In general, the new solution approximation needs to be computed iteratively, typically by a (modified) Newton method, such as

$$x_{n+1}^{(k+1)} = x_{n+1}^{(k)} + \delta x_{n+1}^{(k)}, \quad (2.59)$$

where the increment $\delta x_{n+1}^{(k)}$ is computed by solving a linear system of equations,

$$(\mathbb{1} - hJ_n) \delta x_{n+1}^{(k)} = -r_{n+1}^{(k)}, \quad (2.60)$$

with J_n the Jacobian matrix $Df(t_n, x_n)$ or an approximation to it, and the residual

$$r_{n+1}^{(k)} = x_{n+1}^{(k)} - x_n - hf(t_{n+1}, x_{n+1}^{(k)}). \quad (2.61)$$

The computational cost per step is much larger as with the explicit Euler method. Instead of just a single function evaluation, we now need to compute the Jacobian, solve a linear system and evaluate f on each Newton iteration.

Nevertheless, the implicit Euler method is often preferable over the explicit Euler method, as for many problems the explicit method is only stable for ridiculously small time steps h . In such cases, the implicit Euler method may be cheaper overall as the possibility of taking much larger time steps outweighs the increased cost per time step.

2.3.2 Error and Order

For the explicit Euler method (2.57), the error after one time step starting from the exact solution, called the *local error*, is given as

$$d_{n+1} = (x(t_n) + hf(t_n, x(t_n))) - x(t_n + h). \quad (2.62)$$

By estimating the remainder term in the Taylor expansion of $x(t_n + h)$ at t_n , we can bound d_{n+1} by

$$\|d_{n+1}\| \leq Ch^2, \quad (2.63)$$

with some constant C which only depends on the function f and on bounds of derivatives of the solution $x(t)$.

Since the method advances in each step with the computed values x_n instead of the exact solution values $x(t_n)$, it is important to know how errors, once introduced, are propagated by the method. The global error,

$$e_n = x_n - x(t_n), \quad (2.64)$$

is the sum of the propagated local errors. For the explicit Euler method (2.57), one can show that the global error satisfies

$$\|e_n\| \leq Mh \quad \text{for } t_n \leq T, \quad (2.65)$$

with $M = (e^{(T-t_0)L} - 1)C/L$ where L is the Lipschitz constant. The explicit Euler method thus converges to the exact solution as $h \rightarrow 0$ with nh fixed, but only at first order. That is the global error is proportional to h whereas the local error is proportional to h^2 .

A method is said to have order p if the local error is bounded by Ch^{p+1} , where h is the step size and C . The order is determined by comparing the Taylor expansion of the exact solution and the numerical solution, which for a method of order p should agree up to and including the h^p term. A drawback of the Euler methods is that they are only order 1. There are different ways to increase the order:

- (i) using additional, auxiliary function evaluations in passing from x_n to x_{n+1} (one-step or Runge-Kutta methods),
- (ii) using previously computed solution values x_{n-1} , x_{n-2} , ..., and/or their function values (multistep methods),
- (iii) or using both (general linear methods).

2.3.3 Runge-Kutta Methods

Two ideas underly Runge-Kutta methods [11, 31]. First, use the *Fundamental Theorem of Calculus*,

$$x(t_{n+1}) = x(t_n) + \int_{t_n}^{t_{n+1}} \dot{x}(t) dt, \quad (2.66)$$

with $\dot{x}(t) = f(t, x(t))$, and approximate the integral by some quadrature formula with s nodes c_i and corresponding weights b_i ,

$$x_{n+1} = x_n + h \sum_{i=1}^s b_i \dot{X}_{n,i}, \quad \dot{X}_{n,i} = f(t_n + c_i h, X_{n,i}). \quad (2.67)$$

Second, the internal stage values $X_{n,i} \approx x(t_n + c_i h)$ are determined by another quadrature formula for the integral from 0 to c_i ,

$$X_{n,i} = x_n + h \sum_{j=1}^s a_{ij} \dot{X}_{n,j}, \quad i = 1, \dots, s, \quad (2.68)$$

with the same function values $\dot{X}_{n,j}$ as for x_{n+1} . Such Runge-Kutta methods,

$$X_{n,i} = x_n + h \sum_{j=1}^s a_{ij} f(t_n + c_j h, X_{n,j}), \quad (2.69a)$$

$$x_{n+1} = x_n + h \sum_{j=1}^s b_j f(t_n + c_j h, X_{n,j}), \quad (2.69b)$$

are often summarised in a so-called Butcher tableaux,

$$\begin{array}{c|ccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & & & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array} = \begin{array}{c|c} c & A \\ \hline & b^T \end{array} =, \quad (2.70)$$

which provides a compact way of specifying a given method.

Explicit Runge-Kutta Methods

If the coefficients satisfy $a_{ij} = 0$ for $j \geq i$, then the above sum actually extends only from $j = 1$ to $i - 1$, and hence $X_1, \dot{X}_1, X_2, \dot{X}_2, \dots, X_s, \dot{X}_s$ can be computed explicitly one after the other. The classical Runge-Kutta method of order 4 is given by

$$\begin{array}{c|ccc|cccc} & 0 & & & & & & \\ c & A & & & & & & \\ \hline & b^T & & & & & & \\ \hline & 1/2 & 1/2 & 0 & 1/2 & & & \\ & 1 & 0 & 0 & 1 & & & \\ \hline & & 1/6 & 2/6 & 2/6 & 1/6 & & \end{array} . \quad (2.71)$$

Explicitly, this becomes

$$\begin{aligned} X_{n,1} &= x_n, & \dot{X}_{n,1} &= f(t_n, X_{n,1}), \\ X_{n,2} &= x_n + \frac{1}{2}h\dot{X}_{n,1}, & \dot{X}_{n,2} &= f(t_n + \frac{1}{2}h, X_{n,2}), \\ X_{n,3} &= x_n + \frac{1}{2}h\dot{X}_{n,2}, & \dot{X}_{n,3} &= f(t_n + \frac{1}{2}h, X_{n,3}), \\ X_{n,4} &= x_n + h\dot{X}_{n,3}, & \dot{X}_{n,4} &= f(t_n + h, X_{n,4}), \end{aligned}$$

for the internal stages, and

$$x_{n+1} = x_n + \frac{h}{6}[\dot{X}_{n,1} + 2\dot{X}_{n,2} + 2\dot{X}_{n,3} + \dot{X}_{n,4}],$$

for the final update rule.

Implicit Runge-Kutta Methods

If the coefficients satisfy $a_{ij} = 0$ for $j > i$, then the Runge-Kutta method is linearly implicit and the solution of $X_1, \dot{X}_1, X_2, \dot{X}_2, \dots, X_s, \dot{X}_s$ is given by solving a linear system of equations.

If the coefficients a_{ij} are not vanishing in general, the Runge-Kutta method is nonlinearly implicit and needs to be solved by a (modified) Newton's method or fixed-point iteration.

Partitioned Runge-Kutta Methods

Sometimes a system of ODEs, e.g., Hamilton's equations, naturally exhibit a partitioned form,

$$\dot{x} = f(x, y), \quad \dot{y} = g(x, y). \quad (2.72)$$

In that case it is often advantageous to solve each system with a different Runge-Kutta method, i.e.,

$$X_{n,i} = x_n + h \sum_{j=1}^s a_{ij} f(t_n + c_j h, X_{n,j}, Y_{n,j}), \quad Y_{n,i} = y_n + h \sum_{j=1}^s \widehat{a}_{ij} g(t_n + c_j h, X_{n,j}, Y_{n,j}), \quad (2.73a)$$

$$x_{n+1} = x_n + h \sum_{j=1}^s b_j f(t_n + c_j h, X_{n,j}, Y_{n,j}), \quad y_{n+1} = y_n + h \sum_{j=1}^s \widehat{b}_j g(t_n + c_j h, X_{n,j}, Y_{n,j}), \quad (2.73b)$$

with two different Butcher tableaus. Such integrators are called *partitioned Runge-Kutta methods*.

Collocation Methods

A collocation method based on the nodes $0 \leq c_1 < \dots < c_s \leq 1$ determines a polynomial $p(t)$ of degree at most s , such that $p(t_n) = x_n$ and the differential equation is satisfied at the s points $t_n + c_i h$,

$$\dot{p}(t) = f(t, p(t)) \quad \text{at } t = t_n + c_i h, \quad i = 1, \dots, s. \quad (2.74)$$

The solution approximation at the end-point is then

$$x_{n+1} = p(t_n + h), \quad (2.75)$$

which is taken as the starting value for the next step. Such collocation methods are equivalent to implicit Runge-Kutta methods, the order of which is equal to the order of the underlying interpolatory quadrature rule with nodes c_i . The highest order $2s$ is thus obtained with Gauss nodes.

2.3.4 Linear Multistep Methods

Linear multistep methods are of the form

$$\sum_{j=0}^r \alpha_j x_{n+j} = h \sum_{j=0}^r \beta_j f_{n+j}, \quad (2.76)$$

with $f_i = f(t_i, x_i)$ and $\alpha_r \neq 0$.

2.3.5 General Linear Methods

General Linear methods [11, 40] are multivalue-multistage methods, which can be seen as a hybrid of linear multistep and Runge-Kutta methods. Such methods are usually represented by four matrices, which can be written as a $(s+r) \times (s+r)$ block matrix,

$$\begin{pmatrix} \mathcal{A} & \mathcal{U} \\ \mathcal{B} & \mathcal{V} \end{pmatrix}, \quad (2.77)$$

where s is the number of stages and r the number of input and output values, so that $\mathcal{A} \in \mathbb{R}^{s \times s}$, $\mathcal{U} \in \mathbb{R}^{s \times r}$, $\mathcal{B} \in \mathbb{R}^{r \times s}$, $\mathcal{V} \in \mathbb{R}^{r \times r}$. Denoting the input values by $y_i^{[n]}$ and the output values by $y_i^{[n+1]}$, with $i = 1, \dots, r$, the stages by $Y_i^{[n]}$ and the stage derivatives by $f(Y_i^{[n]})$, with $i = 1, \dots, s$, the method can be written as

$$\begin{pmatrix} Y^{[n]} \\ y^{[n+1]} \end{pmatrix} = \begin{pmatrix} \mathcal{A} & \mathcal{U} \\ \mathcal{B} & \mathcal{V} \end{pmatrix} \begin{pmatrix} h f(Y^{[n]}) \\ y^{[n]} \end{pmatrix}, \quad (2.78)$$

or explicitly as

$$Y_i^{[n]} = \sum_{j=1}^s a_{ij} h f(Y_j^{[n]}) + \sum_{j=1}^r u_{ij} y_j^{[n]}, \quad (2.79a)$$

$$y_i^{[n+1]} = \sum_{j=1}^s b_{ij} h f(Y_j^{[n]}) + \sum_{j=1}^r v_{ij} y_j^{[n]}. \quad (2.79b)$$

2.4 Solving Nonlinear Systems

Any Runge-Kutta method, solving the equation

$$\dot{z} = f(z), \quad (2.80)$$

can be expressed as

$$Z_{n,i} = z_n + h \sum_{j=1}^s a_{ij} f(Z_{n,j}), \quad (2.81)$$

$$z_{n+1} = z_n + h \sum_{j=1}^s b_j f(Z_{n,j}), \quad (2.82)$$

where z_n and z_{n+1} denote the previous and next time step, respectively, and $Z_{n,i}$ are the stages $t_n + c_i h$ of the Runge-Kutta method. The constants c_i , b_i and a_{ij} , are the nodes, the weights, and the coefficients of the method, respectively. When (2.81) constitutes a nonlinear system of equations, which is often the case, we have to use fixed-point or Newton iteration to solve the system. Once a solution for (2.81) is obtained, (2.82) is merely an explicit update.

2.4.1 Fixed-point Iteration

The algorithm of the fixed-point iteration is as simple as it sounds,

$$Z_{n,i}^{k+1} = z_n + h \sum_{j=1}^s a_{ij} f(Z_{n,j}^k), \quad (2.83)$$

where $Z_{n,i}^{k+1}$ and $Z_{n,i}^k$ denote the value of $Z_{n,i}$ at the current and the previous iteration, $k+1$ and k , respectively. Depending on the problem, useful step-out criteria are given by

$$\max_i \frac{r_i^2}{r_0^2} < r_{\text{atol}}^2, \quad \text{or} \quad \sum_i \frac{r_i^2}{r_0^2} < r_{\text{atol}}^2, \quad (2.84)$$

with

$$r_0^2 = \sum_i (Z_{n,i}^0)^2 \quad \text{and} \quad r_i^2 = (Z_{n,i}^{k+1} - Z_{n,i}^k)^2. \quad (2.85)$$

If the components of Z differ by several order of magnitude, more than one normalisation factor r_0 might be necessary. The tolerance r_{atol} can usually be set to 10^{-15} .

2.4.2 Newton's Method

Another standard technique for solving nonlinear systems is Newton's method. If we start close enough to the solution, the convergence rate is at least quadratic. We write the algorithm as

$$F(Z_n) = Z_{n,i} - z_n - h \sum_{j=1}^s a_{ij} f(Z_{n,j}) = 0. \quad (2.86)$$

Often, this can be solved by Newton iteration with analytic Jacobian $\mathcal{J} = F'$, which is determined by computing the variation of F with respect to the Z^n . Then

$$\mathcal{J}(Z_{n+1}^k) \delta Z_{n+1}^{k+1} = -F(Z_{n+1}^k), \quad (2.87)$$

where n denotes the time step and k denotes the Newton iteration, such that

$$Z_{n+1}^{k+1} = Z_{n+1}^k + \delta Z_{n+1}^{k+1}. \quad (2.88)$$

The iteration is stopped when $f(Z_{n+1}^{k+1})$ drops below a given tolerance.

Modified or Approximate Newton Methods

In order to reduce the computational cost of computing the Jacobian, \mathcal{J} is replaced with an approximate Jacobian, e.g., instead of $\mathcal{J}(Z_{n+1}^k)$, often $\mathcal{J}(Z_{n+1}^0)$ can be used without increasing the number of iterations.

2.4.3 Starting Approximations

A vital prerequisite for fast convergence of the iterative solver is a good initial guess. The simplest algorithm for computing an initial guess which is fourth order accurate is Hermite extrapolation.

Hermite extrapolation A simplified version of the Hermite extrapolation algorithm can be implemented as

```
hermite(double z0, double z1, double f0, double f1, double t):

    d = 1/(1+t)
    c = d*(d+2)
    num = c*z0 + d*f0
    den = c

    d = 1/t
    c = d*(d-2)
    num += c*z1 + d*f1
    den += c

    return num/den - z1
```

Here, the parameters $z0$ and $z1$ are the coordinates at the previous two time steps z_{n-1} and z_n , respectively, and $f0$ and $f1$ the corresponding functions $f(z_{n-1})$ and $f(z_n)$. The time t corresponds to the node of the Runge-Kutta stage, that is for $Z_{n,i}$ we use $t = c_i$. The routine returns a fourth-order extrapolation for $Z_{n,i}^0$.

2.4.4 Reducing Rounding Errors

There exist several techniques for reducing rounding errors without too much additional effort, especially for Runge-Kutta methods.

Runge-Kutta Methods

In order to obtain better accuracy and to speed up convergence of the iterative solver, we rewrite the first equation in (2.83) as

$$Y_{n,i} = h \sum_{j=1}^s a_{ij} f(z_n + Y_{n,j}), \quad (2.89)$$

and solve this instead of (2.83). This reduces round-off errors and allows for much smaller tolerances than the original system.

Compensated Summation

In the final update rule (2.82), which now is written as

$$z_{n+1} = z_n + h \sum_{j=1}^s b_j f(z_n + Y_{n,j}), \quad (2.90)$$

one can use compensated summation. This effectively allows us to perform the final update in quadruple precision. The algorithm goes as follows:

$$e^* = e_n + h \sum_{j=1}^s b_j f(z_n + Y_{n,j}), \quad (2.91)$$

$$z_{n+1} = z_n + e^*, \quad (2.92)$$

$$e_{n+1} = e^* + (z_n - z_{n+1}). \quad (2.93)$$

This comes at the price of introducing an additional variable e , which saves the error made in the computation of the coordinates at the next time step, but it reduces error accumulation, which might be especially important for long runtime simulations. The initial error e_0 is set to zero.

3 Some Geometry Background

This section aims at giving a concise overview of the geometric foundations underlying the numerical theory presented later on.

3.1 Smooth Manifolds

The theory of smooth manifolds extends concepts and results of the calculus on Euclidean spaces to more general spaces, which do not possess the structure of a normed vector space. The simplest definition of a manifold \mathcal{M} is a set of points that can be labelled by coordinates, that is to each point q of the manifold we associate a set of m numbers, which are called (local) coordinates of the point q . Locally, manifolds are homeomorphic to the Euclidean space \mathbb{R}^m (see Figure 3.1). That is, there exists a continuous, bijective (one-to-one and onto) map between the manifold \mathcal{M} and the Euclidean space \mathbb{R}^m whose inverse map is also continuous. Globally, however, manifolds might have a much more complicated structure. Therefore it is often not possible to define a global coordinate system on a manifold (think of a circle or a sphere) and one has to find coordinate patches (charts) which together cover the whole manifold.

Definition 3.1. A **chart** (local coordinate system) on a set \mathcal{M} is a pair (\mathcal{U}, ϕ) such that \mathcal{U} is an open subset of \mathcal{M} and ϕ is a one-to-one map from \mathcal{U} onto some open subset of \mathbb{R}^m .

Hence, a chart (\mathcal{U}, ϕ) labels each point q in $\mathcal{U} \subset \mathcal{M}$ by m real numbers,

$$\phi(q) = (x^1(q), x^2(q), \dots, x^m(q)) = (x^\mu(q) \mid 1 \leq \mu \leq m), \quad q \in \mathcal{U}. \quad (3.1)$$

This relation defines m functions x^1, x^2, \dots, x^m , which are called coordinate functions, or simply coordinates, associated with the chart (\mathcal{U}, ϕ) . By slight abuse of notation, we often write $q^\mu = x^\mu(q)$. The fact that ϕ is a one-to-one mapping ensures that two different points of \mathcal{U} differ at least in the value of one of the coordinates.

If the manifold is not globally homeomorphic to \mathbb{R}^n , more than one chart is necessary to cover the whole manifold. A collection of charts $\{(\mathcal{U}_i, \phi_i)\}$ covering the whole manifold is called an atlas

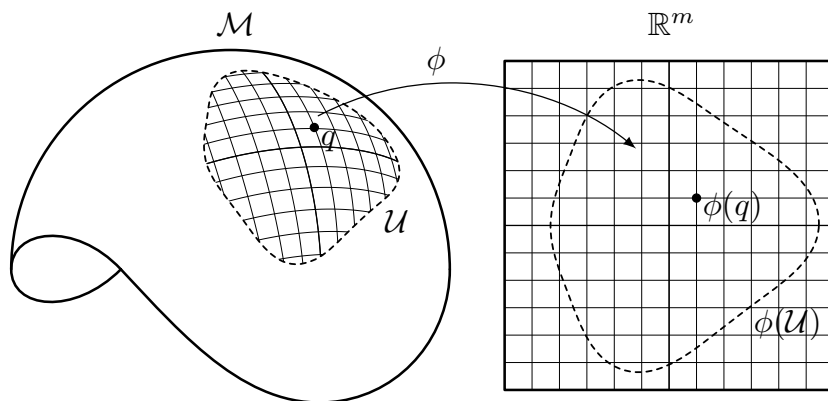


Fig. 3.1: Coordinate chart (\mathcal{U}, ϕ) on a manifold \mathcal{M} .

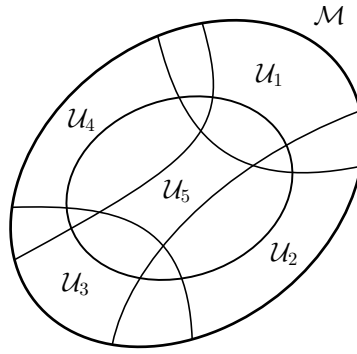


Fig. 3.2: Atlas on a manifold \mathcal{M} consisting of five charts.

(see Figure 3.2). If the atlas consists of more than one chart, some points will lie in the domain of two or more charts and thus have two or more coordinates. In that case, we demand that there exists a transition map, which smoothly maps from one coordinate system to the other as follows.

Definition 3.2. Let (\mathcal{U}_1, ϕ_1) and (\mathcal{U}_2, ϕ_2) be two coordinate patches on \mathcal{M} , overlapping in $\mathcal{U} = \mathcal{U}_1 \cap \mathcal{U}_2 \neq \emptyset$. The composition map

$$\psi = \phi_2 \circ \phi_1^{-1} : \phi_1(\mathcal{U}) \rightarrow \phi_2(\mathcal{U}) \quad (3.2)$$

is called the **transition map** from ϕ_1 to ϕ_2 (see Figure 3.3).

Definition 3.3. Two charts (\mathcal{U}_1, ϕ_1) and (\mathcal{U}_2, ϕ_2) are said to be **smoothly compatible** if either $\mathcal{U}_1 \cap \mathcal{U}_2 = \emptyset$ or the transition map $\psi = \phi_2 \circ \phi_1^{-1}$ is a diffeomorphism.

Definition 3.4. A collection of smoothly compatible charts $\{(\mathcal{U}_i, \phi_i)\}$ whose domains cover all of the manifold \mathcal{M} is called a **smooth atlas** for \mathcal{M} .

Definition 3.5. A **smooth manifold** of dimension m is a set \mathcal{M} with a smooth atlas.

Most manifolds in mathematical physics are smooth manifolds, continuous and infinitely often differentiable. We will always assume that this is the case. If the transition map ψ were not smooth, a function, which is differentiable in one coordinate system, might not be differentiable in

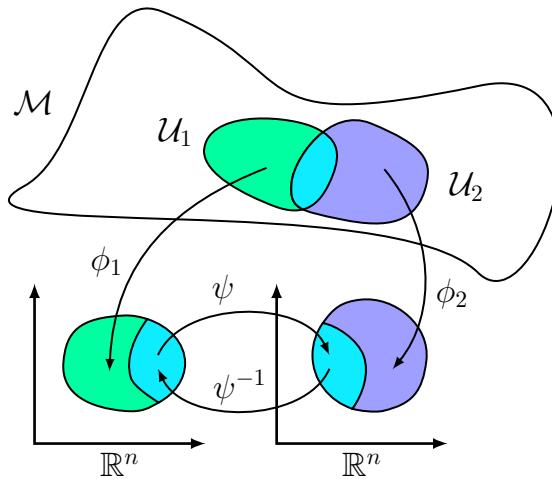


Fig. 3.3: Two charts (\mathcal{U}_1, ϕ_1) and (\mathcal{U}_2, ϕ_2) on a manifold \mathcal{M} .

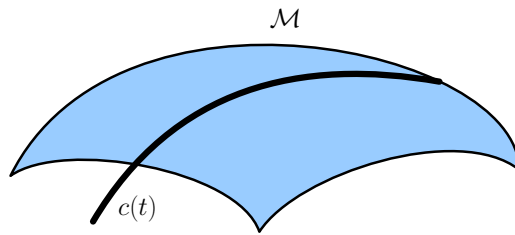


Fig. 3.4: Curve $c(t)$ on a manifold \mathcal{M} .

another coordinate system. Let us remark that most of the definitions and results presented below still hold if we loosen the smoothness requirement to \mathcal{C}^k continuity. Actually, differentiability is usually all we need. However, as we can assume all objects that we encounter in the applications to be smooth, nothing is lost. The smoothness assumption allows us to develop calculus on manifolds in the usual manner and ensures that the results are independent of a particular choice of coordinates. In fact, it turns out that manifolds are the most general spaces on which one can use differential and integral calculus in a similar way as in Euclidean spaces.

In the following, we will also encounter product manifolds. The Cartesian product of two smooth manifolds, \mathcal{M} and \mathcal{N} , acquires the structure of a smooth manifold in a natural way.

Definition 3.6. Let \mathcal{M} be an m -dimensional manifold with atlas $\{(\mathcal{U}_i, \phi_i)\}$ and \mathcal{N} an n -dimensional manifold with atlas $\{(\mathcal{V}_j, \psi_j)\}$. The **product manifold** $\mathcal{M} \times \mathcal{N}$ is a $(m+n)$ -dimensional manifold with atlas $\{(\mathcal{U}_i \times \mathcal{V}_j, \phi_i \times \psi_j)\}$. A point in $\mathcal{M} \times \mathcal{N}$ is denoted by (q, p) with $q \in \mathcal{M}$ and $p \in \mathcal{N}$. The coordinates of (q, p) are $(\phi_i(q), \psi_j(p)) \in \mathbb{R}^{m+n}$.

In Lagrangian mechanics, the configuration space of a mechanical system is a manifold \mathcal{M} . The definition of a coordinate chart on \mathcal{M} amounts to a choice of generalised coordinates. For the cases we will consider, it is always possible to find a global coordinate chart, thereby avoiding the subtleties arising from having more than one coordinate patch. In the remainder of this section we will consider some objects intrinsic to manifolds and basic operations of the calculus on manifolds which will be used in the subsequent treatment.

3.2 Smooth Maps

We will now define curves in manifolds (Figure 3.4), smooth functions on manifolds (Figure 3.5) and smooth maps between manifolds (Figure 3.6).

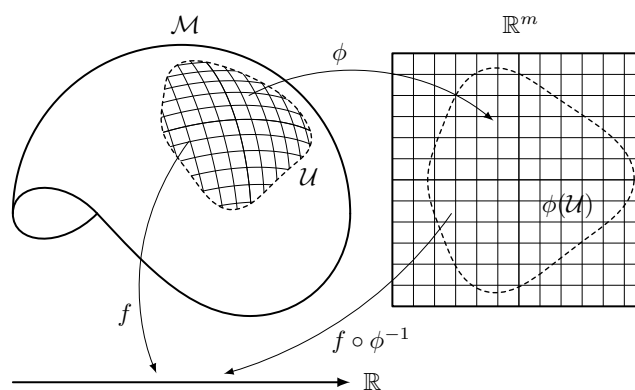


Fig. 3.5: Smooth function f on a manifold \mathcal{M} and its coordinate representation $f \circ \phi^{-1}$.

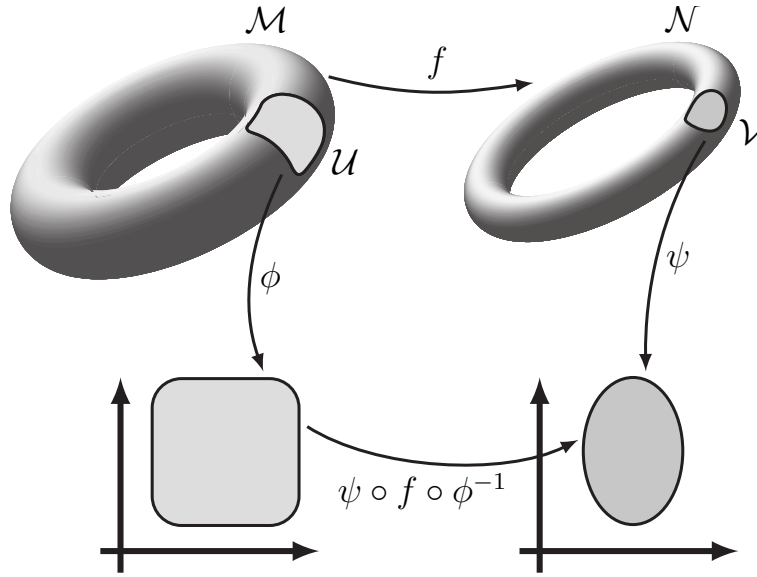


Fig. 3.6: Smooth map f between two manifolds \mathcal{M} and \mathcal{N} and its coordinate representation $\psi \circ f \circ \phi^{-1}$.

Definition 3.7. A **parametrised curve** $c(t)$ in an m -dimensional manifold \mathcal{M} is a smooth map from some interval $\mathcal{I} \subseteq \mathbb{R}$ to the manifold \mathcal{M} ,

$$c: \mathcal{I} \rightarrow \mathcal{M}. \quad (3.3)$$

The function $\phi \circ c: \mathbb{R} \rightarrow \mathbb{R}^m$ is called the **coordinate representation** of $c(t)$ on the chart (\mathcal{U}, ϕ) .

Definition 3.8. Let $f: \mathcal{M} \rightarrow \mathbb{R}$ be a real-valued function defined on a smooth manifold \mathcal{M} . We say that f is a **smooth function** if for every $q \in \mathcal{M}$, there exists a smooth chart (\mathcal{U}, ϕ) for \mathcal{M} such that $q \in \mathcal{U}$ and the coordinate representation $\hat{f} = f \circ \phi^{-1}: \mathbb{R}^m \rightarrow \mathbb{R}$ is smooth on the open subset $\phi(\mathcal{U}) \subseteq \mathbb{R}^m$.

Definition 3.9. Let $f: \mathcal{M} \rightarrow \mathcal{N}$ be a map from an m -dimensional manifold \mathcal{M} to an n -dimensional manifold \mathcal{N} , given by

$$f(q) = (f^1(q), f^2(q), \dots, f^n(q)), \quad (3.4)$$

so that a point $q \in \mathcal{M}$ is mapped to a point $f(q) \in \mathcal{N}$. We say that f is a **smooth map** if for any pair of charts (\mathcal{U}, ϕ) on \mathcal{M} and (\mathcal{V}, ψ) on \mathcal{N} , where $q \in \mathcal{U}$ and $f(q) \in \mathcal{V}$, the coordinate representation $\hat{f} = \psi \circ f \circ \phi^{-1}: \mathbb{R}^m \rightarrow \mathbb{R}^n$ is smooth, i.e., f is smooth if for $q \in \mathcal{M}$ the coordinates of $f(q) \in \mathcal{N}$ depend smoothly on the coordinates of q .

Definition 3.10. A **diffeomorphism** f from a smooth manifold \mathcal{M} to a smooth manifold \mathcal{N} is a smooth bijective map (one-to-one and onto) that has a smooth inverse f^{-1} .

Definition 3.11. Two smooth manifolds \mathcal{M} and \mathcal{N} are said to be **diffeomorphic** if there exists a diffeomorphism between them.

3.3 Vector Fields and the Tangent Bundle

On trivial manifolds, i.e., such manifolds that can be identified with a linear vector space like \mathbb{R}^n , the definition of vector fields is straight forward. Indeed, it is customary to identify points q of

the space \mathbb{R}^n with the corresponding vector $q = (q^1, \dots, q^n)$, leading to the usual notion of vectors. General manifolds, however, are not necessarily linear, so vectors cannot be defined by the usual means. The simplest geometric way to describe a vector v at a point q on a nontrivial manifold is intuitively as the tangent to a parametrised curve $c(t)$ in \mathcal{M} , satisfying $c(0) = q$.

3.3.1 Vectors on Euclidean Spaces

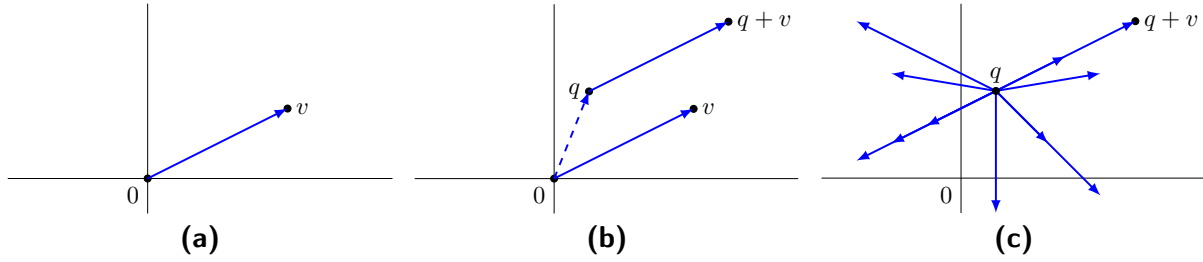


Fig. 3.7: Vectors in Euclidean Spaces.

A vector $v \in \mathbb{R}^n$ is frequently pictured as an arrow from 0 to v (Figure 3.7a). But often, we want to picture the same arrow starting at a different point $q \in \mathbb{R}^n$ (Figure 3.7b). We describe this arrow from q to $q + v$ by the pair (q, v) , sometimes also denoted by v_q (the vector v at point q) or just v , implying the starting point. The set of all such pairs is just $\mathbb{R}^n \times \mathbb{R}^n$, which we will denote by $T\mathbb{R}^n$ and call the tangent bundle of \mathbb{R}^n . Its elements are called tangent vectors.

The vector v at point q is given by the pair (q, v) , but there are many more vectors at q (see Figure 3.7c). The set of all vectors based at the point q is the tangent space to \mathbb{R}^n at q , denoted by $T_q\mathbb{R}^n$ and given by \mathbb{R}^n . The tangent bundle $T\mathbb{R}^n$ of the space \mathbb{R}^n is given by the disjoint union of the tangent spaces to \mathbb{R}^n at all points $q \in \mathbb{R}^n$,

$$T\mathbb{R}^n = \bigcup_{q \in \mathbb{R}^n} T_q\mathbb{R}^n = \mathbb{R}^n \times \mathbb{R}^n. \quad (3.5)$$

The tangent space $T_q\mathbb{R}^n$ corresponds to the derivatives of all possible parametrised curves $c(t)$ in \mathbb{R}^n passing through q . If $c: \mathbb{R} \rightarrow \mathbb{R}^n$ is a differentiable curve, then its derivative $c'(t)$ is just a point of \mathbb{R}^n , but the line between $c(t)$ and $c(t) + c'(t)$ is tangent to the curve and the tangent vector $c'(t)$ is customarily pictured as the arrow from $c(t)$ to $c(t) + c'(t)$. This construction generalises straight forwardly to general manifolds \mathcal{M} as the tangent spaces are always linear vector spaces. However, for the corresponding tangent bundle $T\mathcal{M}$, the cartesian product structure will usually not be present globally but only locally.

3.3.2 Vectors on Manifolds

Consider a smooth curve $c: \mathcal{I} \rightarrow \mathcal{M}$ depending on the parameter t . Assume that we can define a global chart (\mathcal{M}, ϕ) with coordinates denoted by (x^μ) and set $c^\mu(t) = x^\mu(c(t))$, so that the curve can be explicitly written as

$$c: t \mapsto (c^\mu(t)). \quad (3.6)$$

Without loss of generality let us assume that \mathcal{I} contains the point $0 \in \mathbb{R}$ and that $c(0) = q$. We define the tangent vector at $c(0)$ as the directional derivative of a function $f(c(t))$ along the

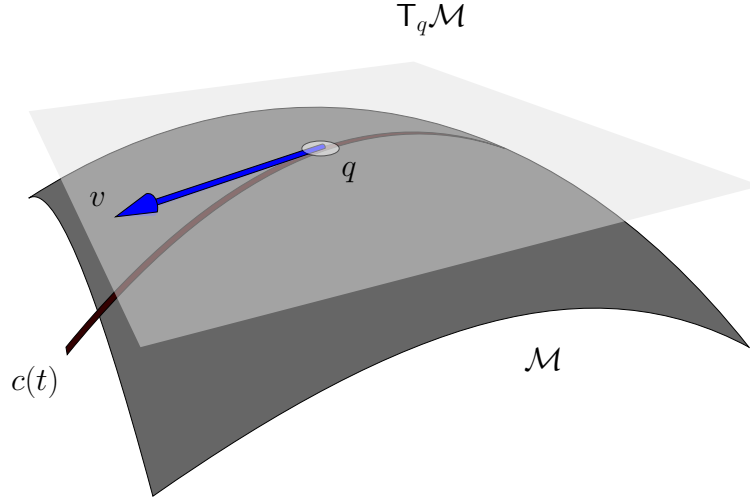


Fig. 3.8: Tangent vector (q, v) to a manifold \mathcal{M} .

curve $c(t)$, where $f : \mathcal{M} \rightarrow \mathbb{R}$, that is

$$v_q(f) = \left. \frac{d}{dt} [f \circ c(t)] \right|_{t=0} = \lim_{t \rightarrow 0} \frac{f(c(t)) - f(c(0))}{t}. \quad (3.7)$$

In terms of local coordinates, this becomes

$$v_q(f) = \frac{dc^\mu}{dt} \frac{\partial \hat{f}}{\partial x^\mu} = \frac{dc^\mu}{dt} \frac{\partial (f \circ \phi^{-1})}{\partial x^\mu}. \quad (3.8)$$

In the literature, $\partial \hat{f} / \partial x^\mu$ is often just written as $\partial f / \partial x^\mu$, implying that the derivative acts on some coordinate representation of f . Equation (3.8) states that we obtain $df(c(t))/dt$ at $t = 0$ by applying the differential operator v_q to f , where

$$v_q = v_q^\mu \partial_\mu \quad \text{with} \quad v_q^\mu \equiv \left. \frac{dx^\mu(c(t))}{dt} \right|_{t=0} \quad \text{and} \quad \partial_\mu \equiv \frac{\partial}{\partial x^\mu}, \quad (3.9)$$

so that v_q^μ are the components of the tangent vector of $c(t)$ at $t = 0$ and ∂_μ are the local basis in which the vector components are expressed. As (3.9) is fully general and independent of f , this constitutes a definition of the tangent vector v_q . In the physics literature, the v_q^μ are usually referred to as contravariant components of the vector v_q .

Mathematically more precise, tangent vectors are defined in terms of equivalence classes of smooth curves on \mathcal{M} . Two curves, $c_1(t)$ and $c_2(t)$, are taken to be equivalent if their first derivative coincides at $t = 0$,

$$c_1(0) = c_2(0) \quad \text{and} \quad \left. \frac{dx^\mu(c_1(t))}{dt} \right|_{t=0} = \left. \frac{dx^\mu(c_2(t))}{dt} \right|_{t=0}, \quad (3.10)$$

in which case we define the equivalence relation $c_1(t) \sim c_2(t)$. If two curves, $c_1(t)$ and $c_2(t)$, are equivalent, they yield the same differential operator v_q at q .

Definition 3.12. The **tangent vector** v_q is identified with the equivalence class of curves given by

$$[c(t)] = \left\{ \tilde{c}(t) \left| \tilde{c}(0) = c(0) = q \quad \text{and} \quad \left. \frac{dx^\mu(\tilde{c}(t))}{dt} \right|_{t=0} = \left. \frac{dx^\mu(c(t))}{dt} \right|_{t=0} \right\}. \quad (3.11)$$

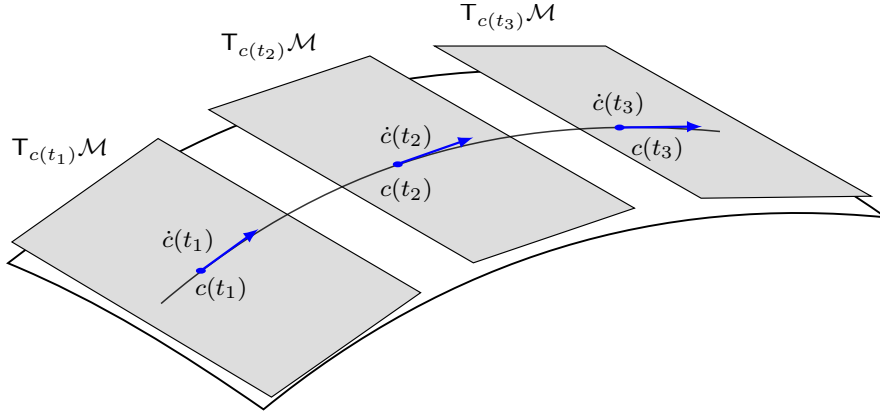


Fig. 3.9: Tangent vectors along a curve $c(t)$ in \mathcal{M} .

Definition 3.13. The **tangent space** $T_q\mathcal{M}$ is defined as the set of all tangent vectors at $q \in \mathcal{M}$.

The tangent space $T_q\mathcal{M}$ at each point $q \in \mathcal{M}$ is a real vector space. It can be thought of as a linear model for the manifold near the point q .

3.3.3 Tangent Bundle

The tangent vector v_q is an element of the local tangent space $T_q\mathcal{M}$, where $T_q\mathcal{M}$ is the set of all tangent vectors (i.e., all possible directional derivatives) to \mathcal{M} at q and has the same dimension as \mathcal{M} . That means, $T_q\mathcal{M}$ can be obtained by considering the tangents to all possible curves passing through the point q . Coordinates (x^μ) on \mathcal{M} induce a basis (∂_μ) on $T_q\mathcal{M}$. Therefore (∂_μ) build a natural coordinate system on $T_q\mathcal{M}$. One possible way of obtaining $T_q\mathcal{M}$ is to consider all possible curves $c(t)$ through q and evaluate (3.9) for each single one.

It is important to note that the tangent vectors to a curve $c(t)$ for different values of t belong to different tangent spaces (see Figure 3.9),

$$(c(t_1), c'(t_1)) \in T_{c(t_1)}\mathcal{M} \neq T_{c(t_2)}\mathcal{M} \ni (c(t_2), c'(t_2)), \quad t_1 \neq t_2. \quad (3.12)$$

As a consequence vectors at different points q_1 and q_2 of the manifold cannot be added or subtracted. This is only possible for vectors at the same point q , i.e., vectors which are elements of the same tangent space $T_q\mathcal{M}$. This motivates the definition of the tangent bundle of a smooth manifold \mathcal{M} in analogy to (3.5), which is obtained by collecting all the $T_q\mathcal{M}$, for each point $q \in \mathcal{M}$, into one single object.

Definition 3.14. The **tangent bundle** $T\mathcal{M}$ is defined as the disjoint union of the tangent spaces to \mathcal{M} at all points $q \in \mathcal{M}$,

$$T\mathcal{M} = \bigcup_{q \in \mathcal{M}} T_q\mathcal{M}. \quad (3.13)$$

The tangent bundle $T\mathcal{M}$ is the set of all tangent vectors at all points of \mathcal{M} and has the structure of a differentiable manifold. Even though tangent vectors $(c(t_1), c'(t_1))$ and $(c(t_2), c'(t_2))$ to a curve $c(t)$ for different parameters t_1 and t_2 belong to different tangent spaces, both vectors belong to the same tangent bundle $T\mathcal{M}$,

$$(c(t), c'(t)) \in T\mathcal{M} \quad \text{for all } t. \quad (3.14)$$

See Figure 3.10 for a pictorial view of the tangent bundle of the circle \mathbb{S}^1 .

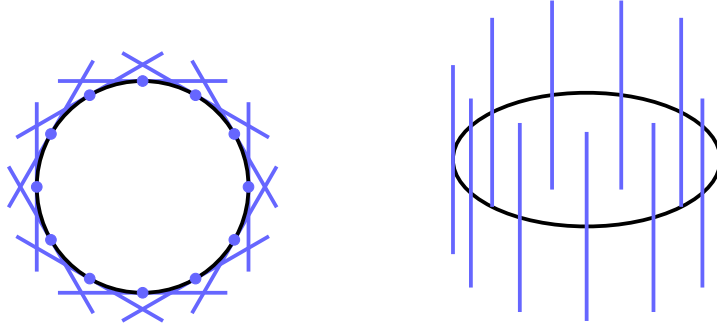


Fig. 3.10: Left: Tangent bundle of the circle \mathbb{S}^1 . Each of the blue lines attached to a point of the circle depicts a fibre of the tangent bundle $T\mathbb{S}^1$. Right: To avoid spurious intersections, the same tangent bundle $T\mathbb{S}^1$ is drawn with the fibres parallel to each other. Now the circle is depicted in the horizontal plane and the fibres $T_q\mathbb{S}^1$ are vertical lines.

3.3.4 Tangent Lifts

Tangent bundles have a natural way of lifting curves and maps in \mathcal{M} to $T\mathcal{M}$.

Definition 3.15. Let \mathcal{M} be a smooth manifold and let coordinates on \mathcal{M} be denoted by (x^μ) . The tangent lift $Tc : \mathcal{I} \rightarrow T\mathcal{M}$ of a curve $c(t) : \mathcal{I} \rightarrow \mathcal{M}$, mapping from some open interval $\mathcal{I} \subseteq \mathbb{R}$ to the manifold \mathcal{M} , is defined by

$$Tc : t \mapsto \left(x^\mu(t), \frac{dx^\mu}{dt}(t) \right). \quad (3.15)$$

Obviously, not every curve in the tangent bundle is the lift of a curve in the base space. Those curves that are lifted ones are called holonomic.

If \mathcal{M} and \mathcal{N} are smooth manifolds, a smooth map $f : \mathcal{M} \rightarrow \mathcal{N}$ induces a linear map of tangent spaces at each point $q \in \mathcal{M}$, called the tangent lift or differential of f at q ,

$$T_q f : T_q \mathcal{M} \rightarrow T_{f(q)} \mathcal{N}, \quad (3.16)$$

as follows.

Definition 3.16. If $V_q \in T_q \mathcal{M}$, then $Tf(V_q)$ is the tangent vector in $T_{f(q)} \mathcal{N}$ defined by

$$(T_q f(V_q))(g) = (Df_q \cdot V_q)(g) = V_q(g \circ f) \in \mathbb{R} \quad \text{for } g \in \mathcal{C}_{f(q)}^\infty(\mathcal{N}). \quad (3.17)$$

The tangent lift $T_q f : T_q \mathcal{M} \rightarrow T_{f(q)} \mathcal{N}$ is a linear map and $T_q f(V_q)$ is a derivation at $f(q)$.

3.3.5 Vector Bundles

The tangent bundle $T\mathcal{M}$ is a particular instance of what is generally referred to as vector bundle. Roughly speaking, a vector bundle over a smooth manifold \mathcal{M} is a collection (or bundle) of vector spaces, one for each point q of \mathcal{M} , that vary smoothly as q varies. Such a vector bundle over \mathcal{M} is a manifold which locally looks like the Cartesian product of \mathcal{M} with a vector space \mathcal{F} , but may possess a different global structure. The vector space \mathcal{F} is usually referred to as the typical fibre. In general, a vector bundle is characterised by four quantities, the base space \mathcal{M} , the total space \mathcal{E} , a typical fibre \mathcal{F} and a projection π . The fibre over some point $q \in \mathcal{M}$, denoted by \mathcal{E}_q is obtained as the preimage of the projection $\pi : \mathcal{E} \rightarrow \mathcal{M}$, i.e., $\mathcal{E}_q = \pi^{-1}(q)$. For the tangent bundle $T\mathcal{M}$, the fibres attached to each point q of the base space \mathcal{M} are the vector spaces $T_q \mathcal{M}$. The points of a single fibre are related to one another while points of different fibres are not.

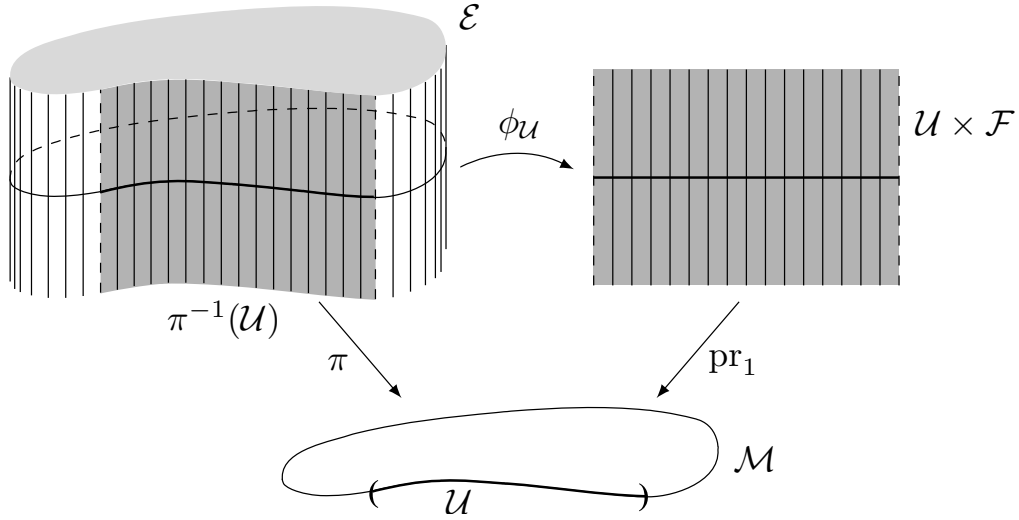


Fig. 3.11: Local trivialization of a vector bundle.

Definition 3.17. A **vector bundle** $(\mathcal{E}, \mathcal{M}, \mathcal{F}, \pi)$ over a manifold \mathcal{M} is a manifold \mathcal{E} and a projection map $\pi : \mathcal{E} \rightarrow \mathcal{M}$ satisfying the following three axioms.

- (a) There exists a vector space \mathcal{F} of dimension m , where m is called the rank of the vector bundle, such that for any point $q \in \mathcal{M}$ the fibre $\mathcal{E}_q = \pi^{-1}(q)$ is a vector space isomorphic to \mathcal{F} .
- (b) For all $q \in \mathcal{M}$ there is an open neighbourhood \mathcal{U} of q and a diffeomorphism

$$\phi_{\mathcal{U}} : \pi^{-1}(\mathcal{U}) \rightarrow \mathcal{U} \times \mathcal{F}, \quad (3.18)$$

such that for every $q \in \mathcal{U}$ the restriction of $\phi_{\mathcal{U}}$ to \mathcal{E}_q ,

$$\phi_{\mathcal{U}}|_{\mathcal{E}_q} : \mathcal{E}_q \rightarrow \{q\} \times \mathcal{F}, \quad (3.19)$$

is a vector space isomorphism and therefore the following diagram commutes,

$$\begin{array}{ccc} \pi^{-1}(\mathcal{U}) & \xrightarrow{\phi_{\mathcal{U}}} & \mathcal{U} \times \mathcal{F} \\ \pi \downarrow & \swarrow \text{pr}_1 & \\ \mathcal{U} & & \end{array}$$

Such an open set \mathcal{U} is called a *trivializing neighbourhood* for \mathcal{E} , and $\phi_{\mathcal{U}}$ is called a *local trivialization* of \mathcal{E} over \mathcal{U} . The map $\text{pr}_1 : \mathcal{U} \times \mathcal{F} \rightarrow \mathcal{U}$ is the projection onto the first factor.

See Figure 3.11 for a schematic of the local trivialization of a vector bundle.

Definition 3.18. For any two maps $\pi : \mathcal{E} \rightarrow \mathcal{M}$ and $\pi' : \mathcal{E}' \rightarrow \mathcal{M}$ with the same target space \mathcal{M} , a map $\phi : \mathcal{E} \rightarrow \mathcal{E}'$ is said to be **fibre-preserving** if $\phi(\mathcal{E}_q) \subset \mathcal{E}'_q$ for all $q \in \mathcal{M}$.

Definition 3.19. A **trivial bundle** is a vector bundle, which is globally a product, $\mathcal{E} = \mathcal{M} \times \mathcal{F}$.

The projection used to construct the tangent bundle (section 3.3.3) and the cotangent bundle (section 3.5.1) is the natural projection.

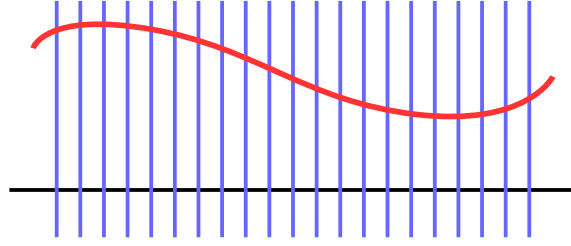


Fig. 3.12: A section in the tangent bundle $T\mathbb{R}$ of the real line.

Definition 3.20. Consider a vector bundle \mathcal{E} over \mathcal{M} , a point q in the base space \mathcal{M} , and the fibre $\mathcal{E}_q \cong \mathcal{F}$ at that point. The **natural projection** π , also referred to as **canonical projection**, maps each element p of \mathcal{E}_q to the point q , the fibre is attached to, i.e.,

$$\pi_{\mathcal{M}} : \mathcal{E} \rightarrow \mathcal{M} \quad (3.20)$$

or in local coordinates

$$\pi_{\mathcal{M}} : (q, p) \mapsto q. \quad (3.21)$$

To avoid confusion, e.g., if more than one projection appears in a treatment, we sometimes also write $\pi_{\mathcal{M}, \mathcal{E}}$ to denote both the source and the target space explicitly. A vector bundle is often just denoted by $\pi_{\mathcal{M}, \mathcal{E}}$ or by $\pi : \mathcal{E} \rightarrow \mathcal{M}$.

Definition 3.21. A **smooth section** φ of a vector bundle \mathcal{E} over \mathcal{M} is a smooth map that assigns to each point q in the base manifold a point in the fibre bundle

$$\varphi : \mathcal{M} \rightarrow \mathcal{E} \quad \text{such that} \quad \pi_{\mathcal{M}, \mathcal{E}} \circ \varphi = \text{id}_{\mathcal{M}}, \quad (3.22)$$

or in local coordinates

$$\varphi : q \mapsto (q, p). \quad (3.23)$$

Sections $\varphi : \mathcal{M} \rightarrow \mathcal{E}$ are also denoted as $\varphi \in \Gamma(\pi_{\mathcal{M}, \mathcal{E}})$, where $\Gamma(\pi_{\mathcal{M}, \mathcal{E}})$ denotes the set of all sections in the vector bundle \mathcal{E} over \mathcal{M} , characterised by the projection $\pi_{\mathcal{M}, \mathcal{E}}$. Note that $\Gamma(\pi_{\mathcal{M}, \mathcal{E}})$ is a vector space (for a proof of the following proposition, see e.g. [73, Page 137]).

Proposition 3.22. Let V and W be smooth sections of a smooth vector bundle $\pi : \mathcal{E} \rightarrow \mathcal{M}$ and let f be a smooth real-valued function on \mathcal{M} . Then

(a) the sum $V + W : \mathcal{M} \rightarrow \mathcal{E}$ defined by

$$(V + W)(q) = V(q) + W(q) \in \mathcal{E}_q, \quad q \in \mathcal{M}, \quad (3.24)$$

is a smooth section of \mathcal{E} .

(b) the product $fV : \mathcal{M} \rightarrow \mathcal{E}$ defined by

$$(fV)(q) = f(q)V(q) \in \mathcal{E}_q, \quad q \in \mathcal{M}, \quad (3.25)$$

is a smooth section of \mathcal{E} .

Remark 3.23. An important generalisation of vector bundles are fibre bundles, where the typical fibre \mathcal{F} is a topological space. If the typical fibre \mathcal{F} is a Lie group, the corresponding fibre bundle is called principle bundle.

3.3.6 Vector Fields

A vector field V on a manifold \mathcal{M} is a function that assigns a tangent vector $V_q \in T_q\mathcal{M}$ to each point $q \in \mathcal{M}$.

Definition 3.24. A **vector field** over \mathcal{M} is a section of the tangent bundle $\pi : T\mathcal{M} \rightarrow \mathcal{M}$.

Consequently, all vector fields V on \mathcal{M} lie in $T\mathcal{M}$ and a vector field V is a linear map

$$V : \mathcal{M} \rightarrow T\mathcal{M}. \quad (3.26)$$

In the following, we provide equivalent definitions of smoothness for vector fields on manifolds. The last one motivates an alternative definition of vector fields.

Definition 3.25. A vector field V is **smooth** if it is a smooth map $\mathcal{M} \rightarrow T\mathcal{M}$.

Lemma 3.26. Let $(\mathcal{U}, \phi) = (\mathcal{U}, x^1, \dots, x^m)$ be a chart on a smooth manifold \mathcal{M} . A vector field $V = v^i \partial/\partial x^i$ on \mathcal{U} is smooth if and only if the coefficient functions v^i are all smooth on \mathcal{U} .

Lemma 3.27. A vector field V is smooth if and only if for every smooth function f on \mathcal{M} , the function $V(f)$ is smooth on \mathcal{M} .

This leads to an alternative definition for vector fields on manifolds.

Definition 3.28. A **vector field** V is a linear map from smooth functions to smooth functions on a manifold \mathcal{M} ,

$$V : \mathcal{C}^\infty(\mathcal{M}) \rightarrow \mathcal{C}^\infty(\mathcal{M}), \quad (3.27)$$

satisfying

$$V(fg) = f(Vg) + g(Vf). \quad (3.28)$$

A vector field V at the point $q \in \mathcal{M}$ is denoted by $V(q)$ or $V|_q$ or just V_q . It is an element of $T_q\mathcal{M}$. As the tangent space $T_q\mathcal{M}$ at each point $q \in \mathcal{M}$ is a real vector space, two vector fields V and W may be point-wise added or multiplied by a scalar field $f : \mathcal{M} \rightarrow \mathbb{R}$ as follows

$$(V + W)(q) = V(q) + W(q), \quad (fV)(q) = f(q)V(q), \quad q \in \mathcal{M}. \quad (3.29)$$

This shows that the set $\mathfrak{X}(\mathcal{M})$ of all smooth vector fields on a manifold \mathcal{M} has the structure of a vector space. This observation is just a special case of Proposition 3.22.

3.4 Integral Curves and Flows

Locally, every smooth vector field may be viewed as the velocity vector field of some flow (like the velocity of a fluid). The path traced out by a point under this flow is called an integral curve of the vector field. Integral curves are curves whose velocity vector field is the restriction of the given vector field to the curve. In that sense, vector fields induce, at least locally, a family of transformations of the manifold onto itself. This topic is essential in the geometric formulation of the theory of ordinary differential equations, the action principle in classical mechanics as well as the study of symmetries with the Noether theorem.

We proceed as follows. First we draw the connection between curves on a manifold \mathcal{M} and one-parameter groups of transformations on \mathcal{M} . Then we show how velocity vector fields of curves relate to generating vector fields of such one-parameter groups of transformations. We will see how this relation can be understood as ordinary differential equations and how solutions of these ODEs constitute integral curves of the generating vector field. Finally, we connect integral curves with the flow of a vector field, thereby closing the circle.

Definition 3.29. A **one-parameter family of transformations** is a smooth map

$$\varphi : \mathcal{M} \times \mathbb{R} \rightarrow \mathcal{M} \quad (3.30)$$

that depends on a real parameter.

A family of transformations is called a group of transformations, if together with any transformation it contains its inverse and for any pair of transformations it also contains their product.

Definition 3.30. A **one-parameter group of transformations** φ on a smooth manifold \mathcal{M} is a smooth map $\varphi : \mathbb{R} \times \mathcal{M} \rightarrow \mathcal{M}$, mapping points of \mathcal{M} to different points of \mathcal{M} ,

$$\varphi : q \mapsto \varphi(q, t) \quad \text{with} \quad q \in \mathcal{M}, \quad t \in \mathbb{R}, \quad (3.31)$$

such that

$$\varphi(q, 0) = q \quad \text{and} \quad \varphi(\varphi(q, s), t) = \varphi(q, s + t) \quad \text{for all} \quad q \in \mathcal{M}, \quad s, t \in \mathbb{R}. \quad (3.32)$$

Upon defining $\varphi_t : \mathcal{M} \rightarrow \mathcal{M}$ by $\varphi_t(q) \equiv \varphi(q, t)$, we can write

$$\varphi_{s+t} = \varphi_s \circ \varphi_t = \varphi_t \circ \varphi_s \quad \text{and} \quad \varphi_0 = \text{id}. \quad (3.33)$$

Each map φ_t has an inverse $\varphi_t^{-1} = \varphi_{-t}$ that is also smooth as

$$\varphi_t \circ \varphi_{-t} = \varphi_{-t} \circ \varphi_t = \varphi_0 = \text{id}. \quad (3.34)$$

Therefore, each φ_t is a diffeomorphism of \mathcal{M} onto itself, and the set of transformations $\{\varphi_t \mid t \in \mathbb{R}\}$ is a group of diffeomorphisms of \mathcal{M} onto itself. Each one-parameter-group of transformations φ on \mathcal{M} determines a family of curves in \mathcal{M} (referred to as the orbits of the group).

Definition 3.31. The **orbit** of an element $q \in \mathcal{M}$ is defined to be the set

$$\varphi_{(q)} = \{\varphi(q, t) \in \mathcal{M} \mid t \in \mathbb{R}\}. \quad (3.35)$$

By some abuse of notation we denote by $\varphi_{(q)}$ also the map $\varphi_{(q)} : \mathbb{R} \rightarrow \mathcal{M}$, given by

$$\varphi_{(q)}(t) = \varphi(q, t), \quad (3.36)$$

which is a differentiable curve in \mathcal{M} for each $q \in \mathcal{M}$. The vector field tangent to these curves generated by the one-parameter-group of transformations is called the infinitesimal generator of φ and defined by

$$V = \left. \frac{d}{dt} \varphi_t \right|_{t=0}. \quad (3.37)$$

For each point $q \in \mathcal{M}$ the above relation defines a vector $V_q = d\varphi_t(q)/dt|_{t=0} \in T_q\mathcal{M}$ with $\varphi_0(q) = q$.

Definition 3.32. Let $\varphi : \mathbb{R} \times \mathcal{M} \rightarrow \mathcal{M}$ be a smooth flow on a smooth manifold \mathcal{M} . The **infinitesimal generator** V to φ is a smooth vector field on \mathcal{M} , such that each curve $\varphi_{(q)}$ with $q \in \mathcal{M}$ is an integral curve of V .

Definition 3.33. Let V be a smooth vector field on a smooth manifold \mathcal{M} and $q \in \mathcal{M}$. An **integral curve** to V is a smooth curve $c : \mathcal{I} \rightarrow \mathcal{M}$, with \mathcal{I} an open interval in \mathbb{R} , $\mathcal{I} \subset \mathbb{R}$, such that $c'(t) = V_{c(t)}$ for all $t \in \mathcal{I}$.

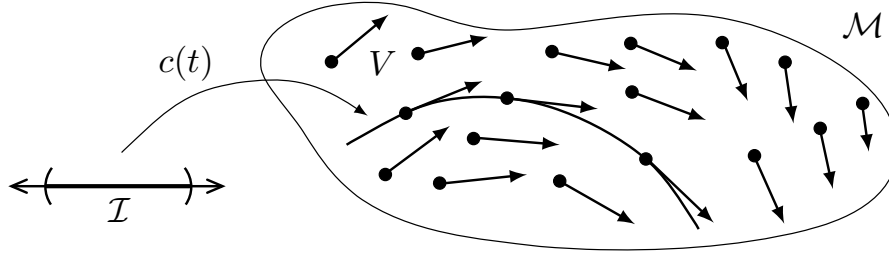


Fig. 3.13: An integral curve $c(t)$ of a vector field V on a manifold \mathcal{M} .

Finding the equation of an integral curve $c(t)$ corresponding to a vector field V is equivalent to solving a system of first-order ordinary differential equations with initial conditions in a smooth chart,

$$\frac{dc^\mu}{dt} = V^\mu(c(t)), \quad c_0^\mu = c^\mu(0), \quad V = V^\mu \frac{\partial}{\partial x^\mu}. \quad (3.38)$$

Let V be a smooth vector field on \mathcal{M} and let $c : \mathcal{I} \rightarrow \mathcal{M}$ be a smooth curve. On a smooth coordinate domain $\mathcal{U} \subseteq \mathcal{M}$, we can write c in local coordinates as $c(t) = (c^1(t), \dots, c^m(t))$. Then the condition $c'(t) = V_{c(t)}$ for c to be an integral curve of V can be written as

$$\dot{c}^\mu(t) \frac{\partial}{\partial x^\mu} \Big|_{c(t)} = V^\mu(c(t)) \frac{\partial}{\partial x^\mu} \Big|_{c(t)}, \quad (3.39)$$

which reduces to the following autonomous system of ordinary differential equations

$$\begin{aligned} \dot{c}^1(t) &= V^1(c^1(t), \dots, c^m(t)), \\ &\vdots \\ \dot{c}^m(t) &= V^m(c^1(t), \dots, c^m(t)), \end{aligned} \quad (3.40)$$

whose simultaneous solution yields the curve $c(t)$. This allows us to reduce the discussion of existence and uniqueness of integral curves on a general manifold \mathcal{M} to the usual theory of ODEs.

Definition 3.34. For any open set \mathcal{U} of \mathcal{M} and any $q \in \mathcal{U}$, we define $c_{(q)}(t)$ to be the integral curve of V through q , with $q = c_{(q)}(0)$. Then the map $\varphi_t : \mathcal{U} \rightarrow \mathcal{M}$ given by $c_{(q)}(0) \mapsto c_{(q)}(t)$ is called the **flow** or the **one-parameter group of diffeomorphisms** of \mathcal{M} generated by the vector field V .

Tangent Lifts of One-Parameter Groups of Diffeomorphisms

If φ_t is a one-parameter group of diffeomorphisms on the base space \mathcal{M} , then $T\varphi_t$ will be a one-parameter group of diffeomorphisms on the tangent bundle $T\mathcal{M}$. Thus, if V is the infinitesimal generator of φ_t , its tangent lift to $T\mathcal{M}$ is given as

$$TV = \frac{d}{dt} T\varphi_t \Big|_{t=0}, \quad (3.41)$$

in local coordinates

$$TV : (x^\mu, V^\mu) \mapsto \left(\left(x^\mu, \frac{dx^\mu}{dt} \right), \left(\frac{dx^\mu}{dt}, \frac{d^2x^\mu}{dt^2} \right) \right). \quad (3.42)$$

The space of such vector fields over $T\mathcal{M}$ plays an important role in the next chapter on Lagrangian dynamics.

3.5 Differential Forms and the Cotangent Bundle

“Very loosely speaking, differential forms are whatever appears under an integral sign.”

- Loring Tu [73]

Somewhat less loosely speaking, they allow us to define integrands over manifolds, thereby providing a natural way to integrate over curved spaces. Just as vector fields, they are intrinsic objects associated to any manifold, and in fact their simplest instance, differential one-forms, are the dual concept to vector fields (which are first order differential operators).

More generally, the calculus of differential forms is a subset of tensor analysis, combining much of the generality of tensors with the simplicity of vectors. Differential k -forms are by far the most useful kind of tensor fields, for several reasons. First, they are easy to define. Second, they are easy to use because, for the most part, one does not have to deal with all those irritating indices. Third, almost all important geometrical quantities can be expressed in terms of forms. And last, but certainly not least, differential forms are essentially the things that appear under integral signs.

3.5.1 Differential One-Forms

A differential one-form α (hereafter just referred to as one-form) is a linear functional that maps vector fields to functions,

$$\alpha : T\mathcal{M} \rightarrow \mathbb{R}. \quad (3.43)$$

A one-form α on a manifold \mathcal{M} assigns an element of the dual space $T_q^*\mathcal{M}$ of the tangent space $T_q\mathcal{M}$ to each point $q \in \mathcal{M}$. It is therefore at the same time a smooth, linear map

$$\alpha : \mathcal{M} \rightarrow T^*\mathcal{M}. \quad (3.44)$$

Each such one-form takes values in the *cotangent space* $T_q^*\mathcal{M}$ at that point, where $T_q^*\mathcal{M}$ contains all dual vectors (covariant vectors) at that point q and has the same dimension as \mathcal{M} . Collecting all the $T_q^*\mathcal{M}$ for each point $q \in \mathcal{M}$ into one single object gives the *cotangent bundle*

$$T^*\mathcal{M} = \bigcup_{q \in \mathcal{M}} T_q^*\mathcal{M}, \quad (3.45)$$

such that the one-form α is a section of $T^*\mathcal{M}$. That way, $T^*\mathcal{M}$ is also the dual to $T\mathcal{M}$. The space $T_q^*\mathcal{M}$ is a vector space, such that two forms α and β of the same degree may be added or multiplied by a scalar field $f : \mathcal{M} \rightarrow \mathbb{R}$

$$(\alpha + \beta)(q) = \alpha(q) + \beta(q), \quad (f\beta)(q) = f(q)\beta(q), \quad q \in \mathcal{M}. \quad (3.46)$$

The simplest geometric way to describe a one-form α is as the differential of a function f on \mathcal{M} . Assume that we can define a global chart (\mathcal{M}, ϕ) with coordinates denoted by (x^μ) and consider a scalar function f on \mathcal{M} . The differential of the function $f : \mathcal{M} \rightarrow \mathbb{R}$ is

$$df = \frac{\partial(f \circ \phi^{-1})}{\partial x^\mu} dx^\mu. \quad (3.47)$$

The first expression on the right-hand side corresponds to the components of the gradient of f , and (dx^μ) forms a local basis, dual to the basis (∂_μ) on $T\mathcal{M}$. However, not all one-forms are differentials of a function. In general, one-forms are written as

$$\alpha = \alpha_\mu dx^\mu. \quad (3.48)$$

The basis (dx^μ) on $T^*\mathcal{M}$ is defined by letting a basis one-form act on a basis vector, i.e.,

$$dx^\mu(\partial_\nu) = \frac{\partial x^\mu}{\partial x^\nu} = \delta_\nu^\mu, \quad (3.49)$$

such that the result of a general one-form α acting on a general vector v is given by

$$\alpha(v) = \alpha_\mu v^\nu \delta_\nu^\mu = \alpha_\mu v^\mu. \quad (3.50)$$

A one-form α is a linear functional, such that it acts on a linear combination of vectors $v, w \in T\mathcal{M}$ with scalars $a, b \in \mathbb{R}$ as

$$\alpha(av + bw) = a\alpha(v) + b\alpha(w). \quad (3.51)$$

In the physics literature, the α_μ are usually referred to as covariant components of the covector field α . Strictly speaking, one-forms can only be identified with covector fields if the underlying manifold is endowed with a metric, which defines a canonical isomorphism of $T_q^*\mathcal{M}$ and $T_q\mathcal{M}$, thus identifying vectors and their duals. In physical applications this is indeed most often the case. To change between vectors and one-forms, the \flat and \sharp operators can be defined like

$$v^\flat = v_i dx^i \quad \text{and} \quad \alpha^\sharp = \alpha^i \partial_i. \quad (3.52)$$

The flat operator \flat returns the one-form corresponding to a vector field, and the sharp operator \sharp returns the vector field corresponding to a one-form. Therefore, the action is the same as in music, but with respect to indices instead of notes.

3.5.2 Differential Two-Forms

A differential two-form ω is a bilinear functional that maps vector fields to functions,

$$\omega : T\mathcal{M} \times T\mathcal{M} \rightarrow \mathbb{R}. \quad (3.53)$$

At the same time, a differential two-form ω is a linear map

$$\omega : \mathcal{M} \rightarrow \bigwedge^2(T^*\mathcal{M}) \quad (3.54)$$

where $\bigwedge^2(T^*\mathcal{M})$ is the vector space of alternating 2-tensors on $T^*\mathcal{M}$. In local coordinates, a two-form ω is generally written¹

$$\omega = \frac{1}{2} \omega_{\mu\nu} dx^\mu \wedge dx^\nu. \quad (3.55)$$

where \wedge denotes the wedge product, which is defined in the next paragraph. Two-forms are antisymmetric, such that

$$\omega_{\mu\nu} = -\omega_{\nu\mu}. \quad (3.56)$$

A similar result as (3.51) holds also for a two-form ω , which is a bilinear functional, acting on vectors $v, w, z \in T\mathcal{M}$ with scalars $a, b \in \mathbb{R}$ as

$$\omega(av + bw, z) = a\omega(v, z) + b\omega(w, z) \quad \text{and} \quad \omega(v, aw + bz) = a\omega(v, w) + b\omega(v, z). \quad (3.57)$$

¹The factor of 1/2 originates from the fact that in the sum over indices all contributions are taken into account twice. Whether it is written or not depends on notational convention.

3.5.3 General Degree Differential Forms

Differential k -forms ξ (differential forms of degree k) are k -linear functionals, mapping k vector fields to functions,

$$\xi : \underbrace{\mathbb{T}\mathcal{M} \times \dots \times \mathbb{T}\mathcal{M}}_{k \text{ times}} \rightarrow \mathbb{R}. \quad (3.58)$$

At the same time, a k -form ξ is a linear map

$$\xi : \mathcal{M} \rightarrow \bigwedge^k \mathbb{T}^* \mathcal{M}, \quad (3.59)$$

where \bigwedge^k is called the k th exterior power of the vector space $\mathbb{T}_q^* \mathcal{M}$, which is the vector space of alternating k -tensors on $\mathbb{T}^* \mathcal{M}$, constructed as

$$\bigwedge^k \mathbb{T}^* \mathcal{M} = \bigcup_{q \in \mathcal{M}} \bigwedge^k \mathbb{T}_q^* \mathcal{M}. \quad (3.60)$$

By definition

$$\bigwedge^1 \mathbb{T}^* \mathcal{M} = \mathbb{T}^* \mathcal{M} \quad \text{and} \quad \bigwedge^0 \mathbb{T}^* \mathcal{M} = \mathbb{R}, \quad (3.61)$$

so that smooth functions on \mathcal{M} are treated as zero-forms. We define the vector space of all k -forms on \mathcal{M} as

$$\Lambda^k(\mathcal{M}) = \Gamma\left(\bigwedge^k \mathbb{T}^* \mathcal{M}\right). \quad (3.62)$$

Differential k -forms are completely covariant, totally antisymmetric tensors. As a consequence of the antisymmetry property, basis forms satisfy

$$dx^\mu \wedge dx^\mu = 0, \quad (3.63)$$

hence the highest degree forms that can exist on a manifold \mathcal{M} of dimension m are of degree m . The generalisation of (3.57) to higher degree forms is straight forward.

Definition 3.35. Let \mathcal{U} be a coordinate patch on \mathcal{M} and let $q \in \mathcal{U}$. A k -form (or a form of degree k) ω_q on \mathcal{U} at q is an element of $\Lambda^k(\mathcal{M})$, in local coordinates given by

$$\omega_q = \frac{1}{k!} \sum a_{i_1 \dots i_k} dx^{i_1} \wedge \dots \wedge dx^{i_k}, \quad (3.64)$$

for some constants $a_l = a_{(i_1 \dots i_l)}$.

Definition 3.36. Let \mathcal{U} be a coordinate patch on \mathcal{M} and let $q \in \mathcal{U}$. A differential k -form ω_q on \mathcal{U} at q is a smooth assignment $q \rightarrow \omega_q$, in local coordinates given by

$$\omega_q = \frac{1}{k!} \sum a_{i_1 \dots i_k}(q) dx^{i_1} \wedge \dots \wedge dx^{i_k}, \quad (3.65)$$

where $a_{(i_1 \dots i_l)}$ are smooth functions on \mathcal{U} .

Example 3.37 (Examples: Differential Forms in a Three-Dimensional Manifold). *1-Form:*

$$A = A_\mu dx^\mu = A_1 dx^1 + A_2 dx^2 + A_3 dx^3 \quad (3.66)$$

2-Form:

$$F = \frac{1}{2} F_{\mu\nu} dx^\mu \wedge dx^\nu = F_{12} dx^1 \wedge dx^2 + F_{23} dx^2 \wedge dx^3 + F_{31} dx^3 \wedge dx^1 \quad (3.67)$$

3-Form:

$$\Omega = \frac{1}{3!} \Omega_{\mu\nu\sigma} dx^\mu \wedge dx^\nu \wedge dx^\sigma = \Omega_{123} dx^1 \wedge dx^2 \wedge dx^3 \quad (3.68)$$

3.5.4 Wedge Product

Definition 3.38. The **wedge product** takes a k -form ξ and a l -form η and returns a $(k+l)$ -form, whose action on $k+l$ vectors (v_1, \dots, v_{k+l}) is given by

$$\xi \wedge \eta(v_1, v_2, \dots, v_{k+l}) = \frac{1}{(k+l)!} \sum_{\sigma \in S_{k+l}} \text{sgn}(\sigma) \xi(v_{\sigma_1}, v_{\sigma_2}, \dots, v_{\sigma_k}) \eta(v_{\sigma_{k+1}}, v_{\sigma_{k+2}}, \dots, v_{\sigma_{k+l}}), \quad (3.69)$$

and which in local coordinates is given by

$$\xi \wedge \eta = \frac{1}{(k+l)!} \sum_{\sigma \in S_{k+l}} \text{sgn}(\sigma) \xi_{\sigma_1, \sigma_2, \dots, \sigma_k} \eta_{\sigma_{k+1}, \sigma_{k+2}, \dots, \sigma_{k+l}} dx^{\sigma_1} \wedge \dots \wedge dx^{\sigma_{k+l}}, \quad (3.70)$$

where $(\sigma_1, \dots, \sigma_k, \sigma_{k+1}, \dots, \sigma_{k+l})$ is an element of S_{k+l} , the group of all permutations of the numbers $\{1, 2, \dots, k+l\}$, and $\text{sgn}(\sigma)$ is the sign of the permutation, i.e.,

$$\text{sgn}(\sigma) = \begin{cases} -1 & \text{odd permutation,} \\ +1 & \text{even permutation.} \end{cases} \quad (3.71)$$

Proposition 3.39. Let ξ , η and σ be differential forms on a smooth manifold \mathcal{M} . Their wedge product has the following properties.

(a) bilinearity:

$$\begin{aligned} (a\xi + b\eta) \wedge \sigma &= a(\xi \wedge \sigma) + b(\eta \wedge \sigma), \\ \xi \wedge (b\eta + c\sigma) &= b(\xi \wedge \eta) + c(\xi \wedge \sigma), \end{aligned} \quad \text{for } a, b, c \in \mathbb{R}, \quad (3.72)$$

(b) associativity:

$$(\xi \wedge \eta) \wedge \sigma = \xi \wedge (\eta \wedge \sigma), \quad (3.73)$$

(c) anticommutativity: for a k -form ξ and a l -form η ,

$$\xi \wedge \eta = (-1)^{kl} \eta \wedge \xi. \quad (3.74)$$

For a proof see e.g. [47, Page 356-357].

Example 3.40 (Examples: Wedge Products of Differential Forms). Consider the examples from above, again defined on a three-dimensional manifold,

$$A = A_1 dx^1 + A_2 dx^2 + A_3 dx^3, \quad (3.75a)$$

$$F = F_{12} dx^1 \wedge dx^2 + F_{23} dx^2 \wedge dx^3 + F_{31} dx^3 \wedge dx^1, \quad (3.75b)$$

$$\Omega = \Omega_{123} dx^1 \wedge dx^2 \wedge dx^3. \quad (3.75c)$$

The wedge product of A with itself is

$$\begin{aligned} A \wedge A &= A_1 A_2 dx^1 \wedge dx^2 + A_2 A_3 dx^2 \wedge dx^3 + A_3 A_1 dx^3 \wedge dx^1 \\ &\quad + A_2 A_1 dx^2 \wedge dx^1 + A_3 A_2 dx^3 \wedge dx^2 + A_1 A_3 dx^1 \wedge dx^3 = 0, \end{aligned} \quad (3.76)$$

which is obvious as by (3.74), for one-forms we have $A \wedge A = -A \wedge A$. The wedge product of A and F is

$$A \wedge F = (A_1 F_{23} + A_2 F_{31} + A_3 F_{12}) dx^1 \wedge dx^2 \wedge dx^3. \quad (3.77)$$

Let us try to compute the wedge product of Ω with the basis forms dx^μ , that is

$$\Omega \wedge dx^1 = \Omega_{123} dx^1 \wedge dx^2 \wedge dx^3 \wedge dx^1 = \Omega_{123} \underbrace{dx^1 \wedge dx^1}_{=0} \wedge dx^2 \wedge dx^3 = 0, \quad (3.78a)$$

$$\Omega \wedge dx^2 = \Omega_{123} dx^1 \wedge dx^2 \wedge dx^3 \wedge dx^2 = -\Omega_{123} dx^1 \wedge \underbrace{dx^2 \wedge dx^2}_{=0} \wedge dx^3 = 0, \quad (3.78b)$$

$$\Omega \wedge dx^3 = \Omega_{123} dx^1 \wedge dx^2 \wedge \underbrace{dx^3 \wedge dx^3}_{=0} = 0. \quad (3.78c)$$

We see that all of these vanish, which is no surprise as Ω is a form of maximum degree.

3.5.5 Interior Product

The interior product of a vector field v and a one-form α is defined as their contraction, denoted

$$\iota_v \alpha = v \lrcorner \alpha = \langle \alpha, v \rangle. \quad (3.79)$$

Definition 3.41. The interior product ι_v is a linear map

$$\iota_v : \Lambda^k(\mathcal{M}) \rightarrow \Lambda^{k-1}(\mathcal{M}), \quad (3.80)$$

taking k -forms ξ into $(k-1)$ -forms $\iota_v \xi$ by

$$\iota_v \xi \left(\underbrace{\dots}_{k \text{ slots}} \right) = \xi \left(v, \underbrace{\dots}_{k-1 \text{ slots}} \right), \quad (3.81)$$

or component-wise

$$\iota_v : \xi_{j_1 j_2 \dots j_k} \mapsto \xi_{i j_2 \dots j_k} v^i. \quad (3.82)$$

The interior product of a vector field v and a scalar function f is zero.

Proposition 3.42. Let $\xi \in \Lambda^k(\mathcal{M})$, $\eta \in \Lambda^l(\mathcal{M})$ and $v \in T\mathcal{M}$. The interior product ι_v is

1. nilpotent

$$\iota_v \circ \iota_v = 0, \quad (3.83)$$

2. an anti-derivation

$$\iota_v(\xi \wedge \eta) = (\iota_v \xi) \wedge \eta + (-1)^k \xi \wedge (\iota_v \eta). \quad (3.84)$$

For a proof see e.g. [47, Pages 358-359] or [73, Pages 227-228]. As an example, consider $v = v^1 \partial_1 + v^2 \partial_2$ and the two-form $dx^1 \wedge dx^2$, so that

$$\iota_v(dx^1 \wedge dx^2) = (\iota_v dx^1) dx^2 - dx^1 (\iota_v dx^2) = v^1 dx^2 - v^2 dx^1. \quad (3.85)$$

3.5.6 Exterior Derivative

The exterior derivative d maps k -forms into $(k+1)$ -forms, thus taking functions (which are considered zero-forms) to one-forms, one-forms to two-forms, and so on. On a three-dimensional manifold, the exterior derivative corresponds to the operators from vector calculus. The exterior derivative of a zero-form corresponds to the gradient, the exterior derivative of a one-form corresponds to the curl, and the exterior derivative of a two-form corresponds to the divergence. On manifolds of dimension other than three, the exterior derivative provides a generalisation of these operators. The exterior derivative is axiomatically defined as follows.

Definition 3.43. The **exterior derivative** d on a manifold \mathcal{M} is a linear map

$$d : \Lambda^k(\mathcal{M}) \rightarrow \Lambda^{k+1}(\mathcal{M}), \quad (3.86)$$

satisfying the following properties. For any k -form ξ and l -form η , the operator d is

(a) linear

$$d(\xi + \eta) = d\xi + d\eta \quad (\text{assuming } k = l) \quad \text{and} \quad d(a\xi) = a d\xi \quad \text{for every } a \in \mathbb{R}, \quad (3.87)$$

(b) a graded derivation (anti-derivation)

$$d(\xi \wedge \eta) = d\xi \wedge \eta + (-1)^k \xi \wedge d\eta \quad (3.88)$$

(c) nilpotent (when applied twice, the exterior derivative vanishes)

$$d^2 = 0 \quad \text{or} \quad d(d\xi) = 0 \quad (3.89)$$

(d) natural: if $f : \mathcal{M} \rightarrow \mathbb{R}$ is a smooth function and v a smooth vector field on \mathcal{M} , then

$$(df)(v) = v(f). \quad (3.90)$$

The last condition states that on zero-forms the exterior derivative df is the ordinary differential of a function f . Hence, in local coordinates (x^μ) ,

$$df = \sum_{\mu} \frac{\partial f}{\partial x^\mu} dx^\mu. \quad (3.91)$$

The vanishing of the exterior derivative when applied twice, $d^2 = 0$, leads to the notion of closed and exact forms.

Definition 3.44. A k -form ξ is **closed** if $d\xi = 0$.

Definition 3.45. A k -form ξ is **exact** if $\xi = d\eta$ for a $(k-1)$ -form η .

Remark 3.46. An exact form is always closed, but a closed form is not necessarily exact.

Example 3.47 (Example: Electromagnetic Field). The natural description of the magnetic potential A is as a one-form

$$A = A_1 dx^1 + A_2 dx^2 + A_3 dx^3. \quad (3.92)$$

The exterior derivative of A ,

$$\begin{aligned} dA &= \left(\frac{\partial A_2}{\partial x^1} - \frac{\partial A_1}{\partial x^2} \right) dx^1 \wedge dx^2 + \left(\frac{\partial A_1}{\partial x^3} - \frac{\partial A_3}{\partial x^1} \right) dx^3 \wedge dx^1 + \left(\frac{\partial A_3}{\partial x^2} - \frac{\partial A_2}{\partial x^3} \right) dx^2 \wedge dx^3 \\ &= \frac{1}{2} (\partial_\mu A_\nu - \partial_\nu A_\mu) dx^\mu \wedge dx^\nu \end{aligned} \quad (3.93)$$

$$\equiv \frac{1}{2} F_{\mu\nu} dx^\mu \wedge dx^\nu, \quad (3.94)$$

yields the magnetic field tensor

$$F = F_{12} dx^1 \wedge dx^2 + F_{23} dx^2 \wedge dx^3 + F_{31} dx^3 \wedge dx^1. \quad (3.95)$$

Interestingly, dA looks like a curl, and indeed, the components of F correspond to the components of the magnetic field $B = \nabla \times A$,

$$F = \begin{pmatrix} 0 & B_3 & -B_2 \\ -B_3 & 0 & B_1 \\ B_2 & -B_1 & 0 \end{pmatrix}. \quad (3.96)$$

Therefore the natural representation of the magnetic field is a two-form. The exterior derivative of F ,

$$dF = \left(\frac{\partial F_{23}}{\partial x^1} + \frac{\partial F_{31}}{\partial x^2} + \frac{\partial F_{12}}{\partial x^3} \right) dx^1 \wedge dx^2 \wedge dx^3, \quad (3.97)$$

does of course vanish as $dF = d^2 A = 0$. Interestingly, dF looks like a divergence and indeed, it corresponds to $\nabla \cdot B = 0$.

3.6 Pullback and Pushforward

Let φ be a diffeomorphism between two smooth manifolds \mathcal{M} and \mathcal{N} ,

$$\varphi : \mathcal{M} \rightarrow \mathcal{N}. \quad (3.98)$$

The map φ allows us to pull back functions and differential forms from the target manifold \mathcal{N} to the source manifold \mathcal{M} as well as to push forward vector fields from \mathcal{M} to \mathcal{N} .

Definition 3.48. The pushforward of a vector field $v : \mathcal{M} \rightarrow T\mathcal{M}$ by φ is a vector field $\varphi_* v : \mathcal{N} \rightarrow T\mathcal{N}$ defined by

$$(\varphi_* v)(\varphi(q)) = D\varphi(q) \cdot v(q) \quad \text{for all } q \in \mathcal{M}. \quad (3.99)$$

Defining local coordinates (x^μ) on \mathcal{M} and (y^μ) on \mathcal{N} , inducing a basis $(\partial/\partial x^\mu)$ on $T\mathcal{M}$ as well as a basis $(\partial/\partial y^\mu)$ on $T\mathcal{N}$, respectively, this can be written as

$$\varphi_* v = v^\nu \frac{\partial \varphi^\mu}{\partial x^\nu} \frac{\partial}{\partial y^\mu}, \quad (3.100)$$

where the matrix $\partial \varphi^\mu / \partial x^\nu$ is just the Jacobian of the map $\varphi : \mathcal{M} \rightarrow \mathcal{N}$.

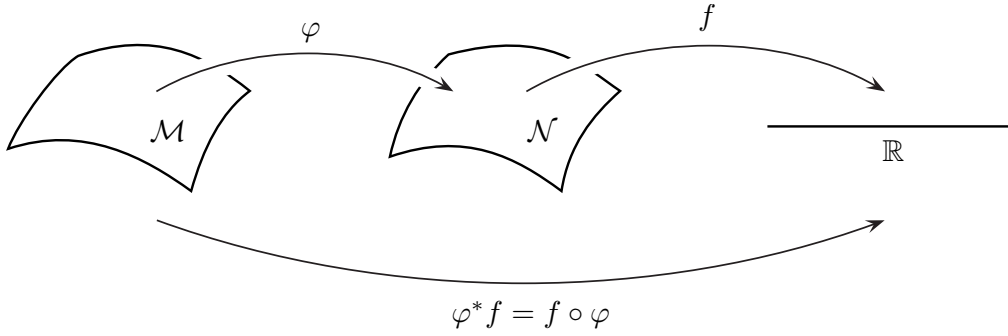


Fig. 3.14: Pullback of a function.

Definition 3.49. The pullback of a smooth function $f : \mathcal{N} \rightarrow \mathbb{R}$ by φ is defined by composition,

$$\varphi^* f = f \circ \varphi. \quad (3.101)$$

The result is a function $\varphi^* f : \mathcal{M} \rightarrow \mathbb{R}$.

Definition 3.50. The pullback of a k -form $\xi \in \Lambda^k(\mathcal{N})$ by φ is defined by

$$(\varphi^* \xi)(v_1, \dots, v_k) = \xi(\varphi_* v_1, \dots, \varphi_* v_k). \quad (3.102)$$

The result is a k -form $\varphi^* \xi \in \Lambda^k(\mathcal{M})$.

While $\varphi^* \xi$ is acting on vectors $v_i \in T_q \mathcal{M}$, ξ is acting on vectors $D\varphi(q) \cdot v_i \in T_{\varphi(q)} \mathcal{N}$, where $1 \leq i \leq k$. The pullback of a wedge product is the wedge product of the pullback

$$\varphi^*(\xi \wedge \eta) = (\varphi^* \xi) \wedge (\varphi^* \eta). \quad (3.103)$$

The pullback of an exterior derivative is the exterior derivative of the pullback

$$\varphi^*(d\xi) = d(\varphi^* \xi) \quad (3.104)$$

where ξ is any differential form.

3.7 Submanifolds

For constraint systems on a smooth manifold \mathcal{M} , the dynamics is usually restricted to a subset $\mathcal{S} \subset \mathcal{M}$ defined by some condition on the dynamical variables like $f(q) = 0$. It is important to know whether or not \mathcal{S} is a smooth manifold itself. This question leads us to the notion of a submanifold.

Definition 3.51. A **submanifold** of \mathcal{M} is a subset $\mathcal{S} \subset \mathcal{M}$ with the property that for each $s \in \mathcal{S}$ there is a chart (\mathcal{U}, φ) in \mathcal{M} with the submanifold property, namely

$$\varphi : \mathcal{U} \rightarrow \mathbb{R}^k \times \mathbb{R}^{m-k} \quad \text{and} \quad \varphi(\mathcal{U} \cap \mathcal{S}) = \varphi(\mathcal{U}) \cap (\mathbb{R}^k \times \{\mathbf{0}\}), \quad (3.105)$$

where k is the dimension of the submanifold and m is the dimension of \mathcal{M} .

This means that if on \mathcal{U} a point $q \in \mathcal{M}$ is labelled by

$$\phi(q) = (x^1(q), x^2(q), \dots, x^m(q)), \quad (3.106)$$

then on $(\mathcal{U} \cap \mathcal{S})$ a point $s \in \mathcal{S}$ is labelled by

$$\varphi(s) = (x^1(s), x^2(s), \dots, x^k(s), 0, \dots, 0). \quad (3.107)$$

A submanifold \mathcal{S} is itself a manifold and all of its charts are of the form $(\mathcal{U} \cap \mathcal{S}, \varphi|_{(\mathcal{U} \cap \mathcal{S})})$ for all charts (\mathcal{U}, φ) of \mathcal{M} which satisfy the submanifold property.

3.8 Lie Groups

In the following, we will encounter Lie groups in various ways. We already discussed one-parameter groups of transformations, which are in fact Lie groups. We will also deal with Lie groups in the analysis of conservation laws of dynamical systems, both on the continuous and the discrete level, where symmetries of the equations of motion with respect to some Lie group implies the conservation of a momentum map. Moreover, there exist systems whose configuration space is modeled on a Lie group, which suggests to use the Lie group structure as a building block for numerical methods.

Definition 3.52. A **group** \mathcal{G} , acting on a set \mathcal{M} , is a set of transformations from \mathcal{M} to \mathcal{M} , such that

- (a) \mathcal{G} includes the identity transformation e , defined by $e \cdot q = q$ for all $q \in \mathcal{M}$,
- (b) \mathcal{G} is closed, i.e., $g_1, g_2 \in \mathcal{G}$ implies $g_1 \circ g_2 \in \mathcal{G}$,
- (c) for each $g \in \mathcal{G}$ there exists $g^{-1} \in \mathcal{G}$, such that $g^{-1} \circ g = e$.

Definition 3.53. A **Lie group** \mathcal{G} is a smooth manifold having a group structure, such that

- (a) the composition \circ is a smooth map $\circ : \mathcal{G} \times \mathcal{G} \rightarrow \mathcal{G}$,
- (b) inversion $\iota(g) = g^{-1}$ is a smooth map $\iota : \mathcal{G} \rightarrow \mathcal{G}$.

Definition 3.54. The **left action** ϕ of a Lie group \mathcal{G} on a smooth manifold \mathcal{M} is a smooth map $\mathcal{G} \times \mathcal{M} \rightarrow \mathcal{M}$, often written as $\phi(g, q) = g \cdot q$ or just $\phi(g, q) = gq$, such that

- (a) $\phi(e, q) = q$ for all $q \in \mathcal{M}$,
- (b) $\phi(h, \phi(g, q)) = \phi(hg, q) = hg \cdot q$ for all $g, h \in \mathcal{G}$ and all $q \in \mathcal{M}$.

Definition 3.55. The **right action** of a group \mathcal{G} on a smooth manifold \mathcal{M} is a smooth map $\mathcal{M} \times \mathcal{G} \rightarrow \mathcal{M}$, often written as $\phi(g, q) = q \cdot g$ or just $\phi(g, q) = qg$, such that

- (a) $\phi(e, q) = q$ for all $q \in \mathcal{M}$,
- (b) $\phi(h, \phi(g, q)) = \phi(gh, q) = q \cdot gh$ for all $g, h \in \mathcal{G}$ and all $q \in \mathcal{M}$.

Remark 3.56. For every $g \in \mathcal{G}$ the map $\phi_g : \mathcal{M} \rightarrow \mathcal{M}$ given by $\phi_g(q) = \phi(g, q)$ is a diffeomorphism with inverse $\phi_g^{-1}(q) = \phi_{g^{-1}}(q)$.

Definition 3.57. If $\phi : \mathcal{G} \times \mathcal{M} \rightarrow \mathcal{M}$ is a (left or right) group action so that $\phi_g : \mathcal{M} \rightarrow \mathcal{M}$ for all $g \in \mathcal{G}$, then the **tangent lift of the group action** $T\phi_g : T\mathcal{M} \rightarrow T\mathcal{M}$ is the corresponding action on the tangent bundle $T\mathcal{M}$ given by

$$(q, v) \mapsto T_q\phi_g(q, v) = (\phi_g(q), T_q\phi_g(v)). \quad (3.108)$$

4 Lagrangian and Hamiltonian Dynamics

We start our journey with Newton's second law,

$$M\ddot{q} = F(q), \quad (4.1)$$

which states that mass times acceleration equals force and provides the equations of motion for a large class of systems from classical mechanics, e.g., systems of point particles. Here, $q = (q^1, \dots, q^d) \in \mathbb{R}^d$ denotes the configuration of some system (e.g., the position of a particle in \mathbb{R}^3), M is a positive-definite symmetric mass matrix (for the particle this is just a scalar m), and F is a force acting on the system. In this chapter, we want to explore what geometric structures are hidden in Newton's equation, thereby laying the foundation for this course. In the following chapters we will discuss various methods of how to preserve these structures in the discretisation. Classical mechanics has two main points of view. *Lagrangian mechanics* and *Hamiltonian mechanics*. In Lagrangian mechanics, the equations of motion,

$$\frac{\partial L}{\partial q}(q(t), \dot{q}(t)) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}}(q(t), \dot{q}(t)) \right) = 0, \quad i = 1, \dots, d, \quad (4.2)$$

referred to as *Euler-Lagrange equations*, are derived from a variational principle, namely *Hamilton's principle of stationary action*. Here, L is called the *Lagrangian*, which is a function of the system's generalised coordinates q and the corresponding generalised velocities \dot{q} . Introducing the generalised momenta $p_i = \partial L / \partial \dot{q}^i$, the Euler-Lagrange equations can be rewritten as a system of first-order ordinary differential equations,

$$\dot{q}^i(t) = \frac{\partial H}{\partial p_i}(q(t), p(t)), \quad \dot{p}_i(t) = -\frac{\partial H}{\partial q^i}(q(t), p(t)), \quad i = 1, \dots, d, \quad (4.3)$$

referred to as *Hamilton equations*. These are the equations of motion of Hamiltonian mechanics, which follow from an energy principle, where H is the total energy of the system and usually referred to as the *Hamiltonian*. The Hamiltonian H is defined by the *Legendre transform* of the Lagrangian and given as a function of the generalised coordinates q^i and the canonical momenta p_i conjugate to the q^i . In both views, different geometric structures take a more prominent role than in the other, albeit all structures are present in both formulations.

The most important of these structures is the so called *symplectic structure*, which is more prominent on the Hamiltonian side. Even though, it has no direct physical meaning, the conservation of the symplectic structure has many practical consequences and is therefore very important in the construction of geometric integration methods.

Another set of important structures are conserved quantities related to symmetries of the Lagrangian or the Hamiltonian with respect to infinitesimal transformations of t or q . These *momenta* or *momentum maps* can be obtained with the help of *Noether's theorem* which is tightly connected to the variational formulation of the equations of motion, so that these structures are more prominent on the Lagrangian side.

4.1 Variational Principle and Euler-Lagrange Equations

At the age of 19, Lagrange found a solution to the long-standing isoperimetric problem¹. As it turned out, more important than the answer to this special problem was Lagrange's solution method, which lead to what we now call the Euler-Lagrange equations (4.2). Some years later, at the age of 18, Hamilton found that these equations can be derived by the principle of stationary action². It states that, considering all possible trajectories $q(t)$ a system could follow to get from a state $q_1 = q(t_1)$ to a state $q_2 = q(t_2)$, the following integral, called the action,

$$\mathcal{A}[q] = \int_{t_1}^{t_2} L(q(t), \dot{q}(t)) dt, \quad (4.4)$$

is stationary for the actual physical trajectory $q(t)$. The action is obtained by integrating the Lagrangian $L(q, \dot{q})$ along a curve $q(t)$. Often, the Lagrangian is given as the difference of kinetic energy $T(\dot{q})$ and potential energy $U(q)$,

$$L(q, \dot{q}) = T(\dot{q}) - U(q). \quad (4.5)$$

For many systems, the kinetic energy is of the form

$$T(\dot{q}) = \frac{1}{2} \dot{q}^T M \dot{q}, \quad (4.6)$$

with M a positive-definite symmetric mass matrix. In order to obtain the Euler-Lagrange equations from the Lagrangian, we apply Hamilton's principle of stationary action, which practically states that the action integral takes a critical point for the physical path, so that at this point infinitesimal variations of the action integral vanish,

$$\delta \mathcal{A}[q] = \delta \int_{t_1}^{t_2} L(q(t), \dot{q}(t)) dt = 0. \quad (4.7)$$

We compute variations of the Lagrangian,

$$\delta \mathcal{A}[q] = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial q}(q(t), \dot{q}(t)) \cdot \delta q + \frac{\partial L}{\partial \dot{q}}(q(t), \dot{q}(t)) \cdot \delta \dot{q} \right] dt = 0, \quad (4.8)$$

where the second term is integrated by parts,

$$\delta \mathcal{A}[q] = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial q}(q(t), \dot{q}(t)) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}}(q(t), \dot{q}(t)) \right) \right] \cdot \delta q dt = 0. \quad (4.9)$$

¹The isoperimetric problem asks, among all closed surfaces of a given fixed perimeter in the plane, which curve maximises the area that it encloses? Lagrange sent his solution to this problem to Euler in 1755.

²Quite often Hamilton's principle is called "principle of least action", which is misleading. In fact, the action does not need to take a minimum but just a critical point. For the derivation of the equations of motion, it doesn't make a difference if the critical point is a minimum, a maximum or a saddle point. Admittedly, most often it is indeed a minimum, but there are counter-examples as well (e.g., under certain conditions the action of the harmonic oscillator takes neither a minimum nor a maximum).

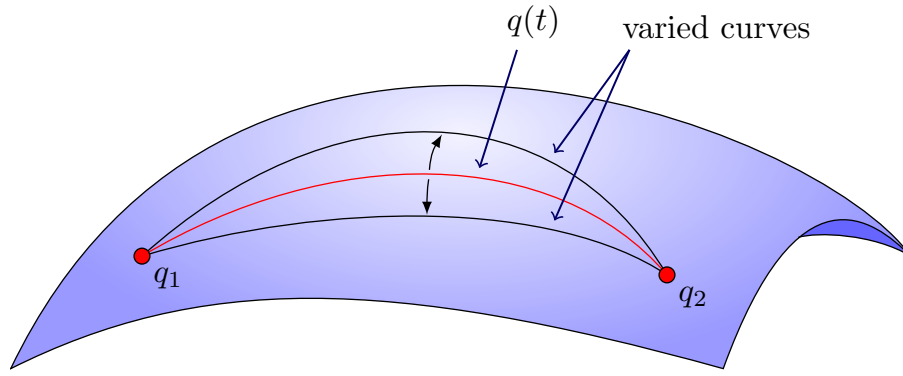


Fig. 4.1: Variations of the Trajectory $q(t)$ with fixed endpoints $q_1 = q(t_1)$ and $q_2 = q(t_2)$.

The boundary terms vanish, as we assume each of the variations of the trajectory to start and end at the same points $q_1 = q(t_1)$ and $q_2 = q(t_2)$ so that $\delta q(t_1) = \delta q(t_2) = 0$ (see Figure 4.1). Further, we assumed that the variation of the time derivative of q equals the time derivative of the variation of q , i.e.,

$$\delta \dot{q} = \frac{d}{dt} \delta q. \quad (4.10)$$

In the present formulation it is not clear why this is justified, but it will become immediate when considering the variations as elements of a one-parameter family of transformations as we will do below. Hamilton's action principle states that q is a critical point of the action if and only if equation (4.9) is satisfied for arbitrary variations δq , only restricted in that they have to vanish at the endpoints. This implies that the expression in square brackets in (4.9) has to vanish. This expression corresponds to the Euler-Lagrange equations (4.2), which are a general statement of Newton's second law for the case of a conservative force field,

$$F(q) = -\nabla U(q). \quad (4.11)$$

Note, however, that also nonconservative forces can be treated in the Lagrangian formalism (see e.g. Jose and Saletan [41, Section 3.3]).

Some Remarks

In introductory textbooks on classical mechanics, the Lagrangian is often defined as a function on the configuration space \mathcal{Q} with coordinates q , which for example might be the three-dimensional euclidean space \mathbb{E}^3 . In that setting, the velocities \dot{q} and accelerations \ddot{q} correspond to the first and second time derivative of q , and if q is a vector in \mathbb{E}^3 , they are as well. The Euler-Lagrange equations are second order differential equations.

This setting, however, does not seem entirely natural. The Lagrangian is defined with respect to q and its first time derivative \dot{q} . So, strictly speaking, L is not a function on \mathcal{Q} but on a larger space, comprising both, coordinates and velocities. Of course, the physics takes place on \mathcal{Q} and embedding it into a larger space is merely a mathematical construct. However, this construct proves to be very useful. So let us take one step back and ask what determines the state of a system. It is not just the position q of all its constituents, but also their respective velocities \dot{q} . We can say that the state of a system corresponds to a point in a state space³ labelled by (q, \dot{q}) . When the system evolves in time, both q and \dot{q} change, and consequently the evolution

³This state space is also called *velocity phase space* in analogy to the *phase space* in Hamiltonian dynamics.

of both, q and \dot{q} , has to be computed, not just the evolution of the coordinates q . It is therefore natural to define the Lagrangian on exactly this space of states. This point of view has many advantages. The obvious one is that the Euler-Lagrange equations become first order differential equations for q and \dot{q} . The consequence of this first order nature of the equations is a separation of the trajectories in state space. There is only one trajectory passing through each point in state space, allowing for the construction of phase portraits. These are visual solutions of the dynamical equations and often useful in the analysis of a dynamical systems' behaviour.

In the next step, these ideas are translated into the geometric language of manifolds. The configuration space is regarded as a smooth manifold, still denoted \mathcal{M} and called the *configuration manifold*, with points labelled by x . The velocity phasespace corresponds to the tangent bundle $T\mathcal{M}$ of that configuration manifold \mathcal{M} , with elements labelled by (x, v) . The Lagrangian therefore comes naturally as a map

$$L : T\mathcal{M} \rightarrow \mathbb{R}. \quad (4.12)$$

The advantage of this point of view might not be apparent if one just thinks in term of Euclidean spaces. It will become clearer considering a particle whose motion is constrained to the two-dimensional surface of a sphere S^2 . The velocity vector of a particle moving in \mathbb{E}^3 is also a vector in \mathbb{E}^3 . In S^2 , however, the velocity vector of a particle is tangent to the sphere. It is not contained in the sphere, but reaches out into the \mathbb{E}^3 in which the sphere is embedded. So to describe the particle motion on S^2 , one has to consider an embedding space. It is not possible to do that only by means of S^2 alone. In this example, there might not be much of an issue, but in other dynamical systems the embedding space might not be so easily found and if it can be found might not have any physical meaning.⁴

Of course, $T\mathcal{M}$ is also a space embedding \mathcal{M} , but in contrast to S^2 and \mathbb{E}^3 , there is an intrinsic relation between \mathcal{M} and $T\mathcal{M}$, given by the tangent lift as discussed in Section 3.3.3, i.e., the tangent bundle $T\mathcal{M}$ is obtained from \mathcal{M} by attaching to each point $x \in \mathcal{M}$ the tangent space $T_x\mathcal{M}$ at that point. The linear space $T_x\mathcal{M}$ contains all possible velocities at x , which are of course tangent to \mathcal{M} at that point.

The Lagrangian maps points (x, v) of $T\mathcal{M}$ to the real numbers \mathbb{R} . The resulting values are completely independent from the coordinates on $T\mathcal{M}$. That way, the description of the dynamics is intrinsic, independent on any particular choice of coordinate systems. Restricting the Lagrangian to solutions of the Euler-Lagrange equations (4.2), it becomes a function of $(q(t), \dot{q}(t))$, as before, but now $q(t)$ refers to the instantaneous value of a curve in \mathcal{M} at time t . In the applications considered later on, it will always be possible to find a global coordinate system for the configuration manifold \mathcal{M} and its tangent bundle $T\mathcal{M}$. This allows to circumvent the issues arising in the case, when the path $q(t)$ and its deformations $q_\epsilon(t)$ are not located in a single coordinate patch⁵.

At this point, a comment is in order. In the literature (as well as the previous section), the arguments of the Lagrangian are often denoted by q and \dot{q} . At the same time, the trajectory on which the Lagrangian is evaluated and the corresponding time derivative are denoted by $q(t)$ and $\dot{q}(t)$. This is both confusing and imprecise. First, there is no distinction between the arguments of the Lagrangian and the element of the domain of the Lagrangian on which it is evaluated. Second, in this notation points of $T\mathcal{M}$ are labelled by (q, \dot{q}) . As the dot usually denotes the time derivative, this notation implies that all curves in $T\mathcal{M}$ are the tangent lift of some curve $q(t)$ in \mathcal{M} . This is of course only true for holonomic curves, e.g., physical trajectories which are solutions $(q(t), \dot{q}(t))$ of the Euler-Lagrange equations (4.2). For general curves $(q(t), v(t))$ on $T\mathcal{M}$ we

⁴See Jose and Saletan [41, section 2.4], for a more detailed discussion.

⁵For a discussion of these issues see Holm, Schmah, and Stoica [36, section 4.1].

have $v \neq dq/dt$. Sometimes, the notation (q, \dot{q}) is used in such a way that \dot{q} does not refer to dq/dt . Then the Euler-Lagrange equations (4.2) take the form

$$\frac{\partial L}{\partial q} \left(q(t), \frac{dq}{dt}(t) \right) - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \left(q(t), \frac{dq}{dt}(t) \right) = 0,$$

which is indeed more precise but also cumbersome and not very natural.

4.1.1 Dynamics on the Tangent Bundle

In this section, we will place the derivation of the Euler-Lagrange equations into a more precise setting. We start by choosing a configuration manifold \mathcal{M} with coordinates $x = (x^1, \dots, x^d)$. The corresponding state space is given by the tangent bundle $T\mathcal{M}$ with induced coordinates $(x, v) = (x^1, \dots, x^d; v^1, \dots, v^d)$. The Lagrangian L is a function on $T\mathcal{M}$,

$$L : T\mathcal{M} \rightarrow \mathbb{R}. \quad (4.13)$$

Consider the space of paths $\mathcal{Q}(\mathcal{M})$ that connect two points in \mathcal{M} ,

$$\mathcal{Q}(\mathcal{M}) = \{q : \mathcal{I} \rightarrow \mathcal{M} \mid \mathcal{I} \subset \mathbb{R} \text{ smooth and bounded, } q \text{ is a } C^2 \text{ curve}\}. \quad (4.14)$$

Fixing two points $q_1, q_2 \in \mathcal{M}$ and an interval $[t_1, t_2] \subset \mathbb{R}$, the path space from q_1 to q_2 is defined as

$$\mathcal{Q}(q_1, q_2, [t_1, t_2]) = \{q : [t_1, t_2] \rightarrow \mathcal{M} \mid q(t_1) = q_1, q(t_2) = q_2\} \subset \mathcal{Q}(\mathcal{M}). \quad (4.15)$$

Elements q of $\mathcal{Q}(q_1, q_2, [t_1, t_2])$ are curves on \mathcal{M} , that is maps that relate points q in configuration space \mathcal{M} to points t in the time interval $[t_1, t_2]$, whereby the first and last points, $q(t_1)$ and $q(t_2)$, take fixed values, q_1 and q_2 , respectively. Consequently, the action can be written as a map

$$\mathcal{A} : \mathcal{Q}(q_1, q_2, [t_1, t_2]) \rightarrow \mathbb{R}, \quad (4.16)$$

assigning real values to each curve $q(t)$ by integrating the Lagrangian L along $q(t)$,

$$\mathcal{A}[q] = \int_{t_1}^{t_2} L(Tq(t)) dt = \int_{t_1}^{t_2} L(q(t), \dot{q}(t)) dt. \quad (4.17)$$

The space of smooth paths $\mathcal{Q}(\mathcal{M})$ can be shown to be a smooth manifold (see Abraham, Marsden, and Ratiu [2]).

4.1.2 Variations as One-Parameter-Families of Transformations

In order to make calculations tractable we do not consider all possible paths from $q(t_1)$ to $q(t_2)$ but a family in which each path is determined by a parameter ϵ . This family shall contain the actual, physical path for $\epsilon = 0$. Such a family of paths constitutes a one-parameter family of transformations. Each path is a function of time, labelled by ϵ ,

$$q_\epsilon(t) \equiv q(t, \epsilon) \quad \text{with fixed } \epsilon. \quad (4.18)$$

The function $q_\epsilon(t)$ shall be differentiable for both, t at fixed ϵ and ϵ at fixed t , such that mixed partial derivatives can be exchanged

$$\frac{\partial^2 q_\epsilon}{\partial t \partial \epsilon} = \frac{\partial^2 q_\epsilon}{\partial \epsilon \partial t}. \quad (4.19)$$

All paths shall start at $q(t_1)$ and end at $q(t_2)$, such that

$$\begin{aligned} q_\epsilon(t_1) &= q_0(t_1) = q(t_1) \equiv q_1 \\ q_\epsilon(t_2) &= q_0(t_2) = q(t_2) \equiv q_2 \end{aligned} \quad (4.20)$$

or

$$\frac{\partial q_\epsilon}{\partial \epsilon}(t_1) = \frac{\partial q_\epsilon}{\partial \epsilon}(t_2) = 0. \quad (4.21)$$

One example of such a family, often considered exclusively in classical mechanics textbooks, is

$$q_\epsilon(t) = q(t) + \epsilon \delta q. \quad (4.22)$$

This, however, requires that $q(t)$ takes values in a linear space, an assumption that generally cannot be made in the geometric framework on manifolds. Therefore we consider more general transformations of the form (4.18).

The generating vector field of such a transformation is called an infinitesimal variation of q and living in the tangent space $T_q \mathcal{Q}(q_1, q_2, [t_1, t_2])$ of $\mathcal{Q}(q_1, q_2, [t_1, t_2])$ at q . The tangent vector to some path $q_\epsilon \in \mathcal{Q}(q_1, q_2, [t_1, t_2])$ is given by

$$V(t) = \left. \frac{d}{d\epsilon} q_\epsilon(t) \right|_{\epsilon=0}. \quad (4.23)$$

For each fixed t , q_ϵ is a curve in \mathcal{M} through the point $q_0(t) = q(t)$, such that $V(t)$ is a tangent vector to \mathcal{M} based at $q(t)$, i.e., $V(t) \in T_{q(t)} \mathcal{M}$ and thus $\pi_{\mathcal{M}} \circ V = q$, where $\pi_{\mathcal{M}} : T\mathcal{M} \rightarrow \mathcal{M}$. From the restrictions $q_\epsilon(t_1) = q_1$ and $q_\epsilon(t_2) = q_2$ follows that $V(t_1) = 0$ and $V(t_2) = 0$, but otherwise V is an arbitrary C^2 map.

Definition 4.1. The *infinitesimal variation* of a path $q : [t_1, t_2] \rightarrow \mathcal{M}$, is the set of C^2 maps

$$V : [t_1, t_2] \rightarrow T\mathcal{M} \quad \text{for which} \quad \pi_{\mathcal{M}} \circ V = q \quad \text{and} \quad V(t_1) = 0, \quad V(t_2) = 0. \quad (4.24)$$

Definition 4.2. The *tangent space* to $\mathcal{Q}(q_1, q_2, [t_1, t_2])$ at the curve $q \in \mathcal{Q}(q_1, q_2, [t_1, t_2])$ is given as follows,

$$\begin{aligned} T_q \mathcal{Q}(q_1, q_2, [t_1, t_2]) &= \{ V : [t_1, t_2] \rightarrow T\mathcal{M} \mid V \text{ is a } C^2 \text{ map,} \\ &\quad \pi_{\mathcal{M}} \circ V = q, \quad V(t_1) = 0, \quad V(t_2) = 0 \}. \end{aligned} \quad (4.25)$$

Remark 4.3. The usual notation is recovered by defining

$$\delta \equiv \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \quad (4.26)$$

and calling $V = \delta q$ an infinitesimal variation of the path $q(t)$ with fixed endpoints.

Remark 4.4. By the above arguments, especially equations (4.19) and (4.26), it is clear that the variation of the time derivative of q equals the time derivative of the variation of q , i.e.,

$$\delta \dot{q} = \frac{d}{dt} \delta q, \quad (4.27)$$

an important point that is often obfuscated by oversimplification.

4.1.3 Hamilton's Principle of Stationary Action

If L is the Lagrangian on $\mathcal{T}\mathcal{M}$ and $q(t)$ is a path $q : [t_1, t_2] \rightarrow \mathcal{M}$ that connects $q_1 = q(t_1)$ with $q_2 = q(t_2)$, then inserting the tangent lift $\mathcal{T}q = (q, \dot{q})$ of this path q into the Lagrangian, $L(q(t), \dot{q}(t))$, it becomes a function of time only. This time dependency is different for all the possible paths q , such that the action integral $\mathcal{A}[q]$ takes different values for different paths q and

$$\mathcal{A}[q_\epsilon] = \int_{t_1}^{t_2} L(q_\epsilon(t), \dot{q}_\epsilon(t)) dt \quad (4.28)$$

takes different values for different ϵ . Hamilton's principle of stationary action states that a path q obeys the Euler-Lagrange equations,

$$\frac{\partial L}{\partial x}(q(t), \dot{q}(t)) = \frac{d}{dt} \frac{\partial L}{\partial v}(q(t), \dot{q}(t)), \quad (4.29)$$

if and only if q is a critical point of the function $\mathcal{A} : \mathcal{Q}(q_1, q_2, [t_1, t_2]) \rightarrow \mathbb{R}$ or in other words if \mathcal{A} is stationary for q . Stationarity of $\mathcal{A}[q]$ means that $\mathcal{A}[q]$ does not change under infinitesimal variations of the path q so that $\delta\mathcal{A}[q] = 0$.

For each one-parameter family q_ϵ that satisfies the above conditions (4.19)-(4.21), a path q is a critical point of the action \mathcal{A} if and only if

$$\delta\mathcal{A}[q] = \left. \frac{d}{d\epsilon} \mathcal{A}[q_\epsilon] \right|_{\epsilon=0} = 0. \quad (4.30)$$

With the chain rule one obtains

$$\left. \frac{d}{d\epsilon} \mathcal{A}[q_\epsilon] \right|_{\epsilon=0} = \frac{\partial \mathcal{A}}{\partial x}[q] \cdot \left. \frac{dq_\epsilon}{d\epsilon} \right|_{\epsilon=0} = d\mathcal{A}[q] \cdot V, \quad (4.31)$$

where $d\mathcal{A}[q]$ and $V = dq_\epsilon/d\epsilon|_{\epsilon=0}$ are regarded as elements of the cotangent and tangent spaces $\mathcal{T}_q^*\mathcal{Q}$ and $\mathcal{T}_q\mathcal{Q}$ on the manifold \mathcal{Q} , respectively. Therefore the variation of the action can be formulated as

$$d\mathcal{A}[q] \cdot V = \left. \frac{d}{d\epsilon} \left[\int_{t_1}^{t_2} L(q_\epsilon(t), \dot{q}_\epsilon(t)) dt \right] \right|_{\epsilon=0}, \quad (4.32)$$

where L is evaluated on the tangent lift of q_ϵ ,

$$\mathcal{T}q_\epsilon : t \mapsto (q_\epsilon(t), \dot{q}_\epsilon(t)). \quad (4.33)$$

The derivative⁶ $\dot{q}_\epsilon \equiv dq_\epsilon/dt$ is the generalised velocity along a particular trajectory that is labelled by a specific value of ϵ . The integration limits are fixed, so that the ϵ -derivative can be moved under the integral,

$$d\mathcal{A}[q] \cdot V = \int_{t_1}^{t_2} \left. \frac{d}{d\epsilon} \left[L(q_\epsilon, \dot{q}_\epsilon) \right] \right|_{\epsilon=0} dt = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial x}(q, \dot{q}) \cdot \left. \frac{dq_\epsilon}{d\epsilon} \right|_{\epsilon=0} + \frac{\partial L}{\partial v}(q, \dot{q}) \cdot \left. \frac{d\dot{q}_\epsilon}{d\epsilon} \right|_{\epsilon=0} \right] dt, \quad (4.34)$$

⁶As the time derivative \dot{q}_ϵ is taken for fixed ϵ , it should better be denoted $\partial q_\epsilon / \partial t$. However, the important point is that the derivatives with respect to time t and with respect to ϵ can be exchanged as in (4.19) such that integration by parts can be performed.

which leads to

$$d\mathcal{A}[q] \cdot V = \int_{t_1}^{t_2} dL(q, \dot{q}) \cdot TV dt = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial x}(q, \dot{q}) \cdot V + \frac{\partial L}{\partial v}(q, \dot{q}) \cdot \dot{V} \right] dt, \quad (4.35)$$

with (V, \dot{V}) the tangent lift of the generating vector field V ,

$$TV : (q, V) \mapsto ((q, V), (\dot{q}, \dot{V})). \quad (4.36)$$

Because of (4.19), the second term on the right-hand side can be integrated by parts, leading to

$$d\mathcal{A}[q] \cdot V = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial x}(q, \dot{q}) - \frac{d}{dt} \left(\frac{\partial L}{\partial v}(q, \dot{q}) \right) \right] \cdot V dt + \left[\frac{\partial L}{\partial v}(q, \dot{q}) \cdot V \right]_{t_1}^{t_2}. \quad (4.37)$$

The last term vanishes as V vanishes on both ends of the trajectory, c.f. (4.24), such that

$$d\mathcal{A}[q] \cdot V = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial x}(q, \dot{q}) - \frac{d}{dt} \left(\frac{\partial L}{\partial v}(q, \dot{q}) \right) \right] \cdot V dt. \quad (4.38)$$

The requirement $\delta\mathcal{A}[q] = 0$ is equivalent to $d\mathcal{A}[q] \cdot V = 0$ for all $V \in T_q\mathcal{Q}(q_1, q_2, [t_1, t_2])$ as well as to the Euler-Lagrange equations (4.29), as V is an arbitrary function of time, only restricted in that it has to vanish at the end points of the trajectory⁷.

Definition 4.5. A curve $q \in \mathcal{Q}(q_1, q_2, [t_1, t_2])$ is said to be a **solution of the Euler-Lagrange equations** (4.29) if the right-hand side of (4.38) vanishes for arbitrary variations $V \in T_q\mathcal{Q}(q_1, q_2, [t_1, t_2])$.

4.1.4 Euler-Lagrange Operator

The Euler-Lagrange equations are defined on the second-order submanifold $\ddot{\mathcal{M}}$, which is simply the set of second-order derivatives $\ddot{q}(0)$ of curves $q : \mathcal{I} \rightarrow \mathcal{M}$, which are of the form $((q, \dot{q}), (\dot{q}, \ddot{q})) \in T(T\mathcal{M})$.

Definition 4.6. The **second-order submanifold** of $T(T\mathcal{M})$ is defined to be

$$\ddot{\mathcal{M}} = \{w \in T(T\mathcal{M}) \mid T\pi_{\mathcal{M}}(w) = \pi_{T\mathcal{M}}(w)\} \subset T(T\mathcal{M}), \quad (4.39)$$

where $\pi_{T\mathcal{M}} : T(T\mathcal{M}) \rightarrow T\mathcal{M}$ and $\pi_{\mathcal{M}} : T\mathcal{M} \rightarrow \mathcal{M}$ are the canonical projections on $T(T\mathcal{M})$ and $T\mathcal{M}$, respectively.

$$\begin{array}{ccc} T\mathcal{M} & \xleftarrow{\pi_{T\mathcal{M}}} & T(T\mathcal{M}) \\ \pi_{\mathcal{M}} \downarrow & & \uparrow T\pi_{\mathcal{M}} \\ \mathcal{M} & & \end{array}$$

⁷For a deeper discussion of this point see e.g. Arnold [3, Section 12], Gelfand and Fomin [27, Section 3] or Hunter and Nachtergaele [37, Section 13.7].

This states that $\ddot{\mathcal{M}}$ contains those elements of $T(T\mathcal{M})$ for which the two projections $\pi_{T\mathcal{M}}$ and $T\pi_{\mathcal{M}}$ coincide. To see what that means, write out both expressions, that is

$$\pi_{T\mathcal{M}} : ((x, v), (w, a)) \mapsto (x, v), \quad (4.40a)$$

$$T\pi_{\mathcal{M}} : ((x, v), (w, a)) \mapsto (x, w). \quad (4.40b)$$

Requiring that both projections are equivalent therefore means singling out those elements of $T(T\mathcal{M})$ for which $v = w$. These correspond to curves $q(t) \in \mathcal{M}$ which are tangent lifted twice, first to $T\mathcal{M}$, then to $T(T\mathcal{M})$. In other words, elements $w \in \ddot{\mathcal{M}}$ are those elements of $T(T\mathcal{M})$ that are of the form

$$w = ((q, \dot{q}), (\dot{q}, \ddot{q})). \quad (4.41)$$

An alternative definition of the second order submanifold $\ddot{\mathcal{M}}$ is therefore

$$\ddot{\mathcal{M}} = \left\{ \frac{d^2 q}{dt^2}(0) \in T(T\mathcal{M}) \mid q(t) \text{ a curve in } \mathcal{M} \right\} \subset T(T\mathcal{M}). \quad (4.42)$$

Given a Lagrangian L , there exists a map on $\ddot{\mathcal{M}}$,

$$D_{\text{EL}} L : \ddot{\mathcal{M}} \rightarrow T^*\mathcal{M}, \quad (4.43)$$

referred to as the Euler-Lagrange map. It defines a one-form in the dual space $T^*\mathcal{M}$ of $T\mathcal{M}$, given by

$$D_{\text{EL}} L = \frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial v}. \quad (4.44)$$

It is a function on $\ddot{\mathcal{M}} \subset T(T\mathcal{M})$ as

$$D_{\text{EL}} L(\ddot{q}(t)) = \frac{\partial L}{\partial x}(q(t), \dot{q}(t)) - \frac{\partial^2 L}{\partial v \partial x}(q(t), \dot{q}(t)) \cdot \dot{q}(t) - \frac{\partial^2 L}{\partial v \partial v}(q(t), \dot{q}(t)) \cdot \ddot{q}(t). \quad (4.45)$$

With that, the Euler-Lagrange equations can be rewritten as $D_{\text{EL}} L(\ddot{q}(t)) = 0$, implying that by slight abuse of notation $\ddot{q} = ((q, \dot{q}), (\dot{q}, \ddot{q}))$. The covariance of the Euler-Lagrange equation, first observed in the original work of Lagrange, is obtained here as a natural consequence of the geometric framework.

4.1.5 Lagrangian Vector Fields and Flows

Definition 4.7. The **Lagrangian vector field** $X_L : T\mathcal{M} \rightarrow \ddot{\mathcal{M}}$ is a second-order vector field on $T\mathcal{M}$ satisfying

$$D_{\text{EL}} L \circ X_L = 0, \quad (4.46)$$

and the **Lagrangian flow** $F_L : T\mathcal{M} \times \mathbb{R} \rightarrow T\mathcal{M}$ is the flow of X_L .

We will write $F_L^t : T\mathcal{M} \rightarrow T\mathcal{M}$ for the map F_L at the frozen time t . For an arbitrary Lagrangian L , equation (4.46) may not uniquely define the vector field X_L and hence the flow map F_L may not exist.

Theorem 4.8. Given a Lagrangian $L : T\mathcal{M} \rightarrow \mathbb{R}$, the Lagrangian vector field X_L , and hence the Lagrangian flow map F_L are well-defined if and only if the Lagrangian is regular, i.e.,

$$\left| \frac{\partial^2 L}{\partial v^i \partial v^j}(q, \dot{q}) \right| \neq 0. \quad (4.47)$$

Theorem 4.9. The tangent lift $Tq : t \mapsto (q(t), \dot{q}(t))$ of a curve $q \in \mathcal{Q}(q_1, q_2, [t_1, t_2])$ is an integral curve of X_L if and only if q satisfies the Euler-Lagrange equations (4.29) for all $t \in (t_1, t_2)$.

4.2 From the Lagrangian to the Hamiltonian

In the Hamiltonian formulation of classical mechanics, the generalised velocities are replaced with generalised momenta and the dynamics takes place on the cotangent bundle $T^*\mathcal{M}$ instead of the tangent bundle $T\mathcal{M}$. Hamilton's equations of motion constitute a set of first-order differential equations on $T^*\mathcal{M}$ which exhibit far greater symmetry than the Euler-Lagrange equations on $T\mathcal{M}$. As a result, the presence of some geometric structures is quite evident in the Hamiltonian formulation while being rather hidden in the Lagrangian formulation. Most importantly, $T^*\mathcal{M}$ has a natural symplectic structure which is not the case for $T\mathcal{M}$. In the following, coordinates on $T^*\mathcal{M}$ are denoted by (x, p) , while curves in $T^*\mathcal{M}$ are denoted by (q, p) .

4.2.1 Legendre Transform

The canonical momenta p_i conjugate to q^i , are defined as

$$p_i = \frac{\partial L}{\partial v^i}(q, v). \quad (4.48)$$

This transformation constitutes what is called a fibre derivative,

$$\mathbb{F}L : T\mathcal{M} \rightarrow T^*\mathcal{M}, \quad (4.49)$$

globally defined as the derivative of L in each fibre $T_q\mathcal{M}$ of $T\mathcal{M}$,

$$\mathbb{F}L(v) \cdot w = \left. \frac{d}{d\epsilon} L(v + \epsilon w) \right|_{\epsilon=0}, \quad v, w \in T_q\mathcal{M}, \quad (4.50)$$

and locally given by

$$\mathbb{F}L : (q, v) \mapsto \left(q, \frac{\partial L}{\partial v}(q, v) \right). \quad (4.51)$$

The fibre derivative is a fibre-preserving mapping, that is it maps fibres of $T\mathcal{M}$ into fibres of $T^*\mathcal{M}$. If the fibre derivative $\mathbb{F}L$ is a local diffeomorphism, the Lagrangian L is called regular. If $\mathbb{F}L$ is a global diffeomorphism, the Lagrangian L is called hyperregular. Denote by \mathcal{H} the Hessian of the map $v \mapsto L(q, v)$ for fixed q , that is a symmetric bilinear form on $T_q\mathcal{M}$. Hyperregularity of the Lagrangian is equivalent to Legendre's condition that the Hessian \mathcal{H} is nondegenerate, i.e.,

$$\det \mathcal{H} = \det \left| \frac{\partial^2 L}{\partial v^i \partial v^j}(q, v) \right| \neq 0, \quad \text{for all } q \in \mathcal{M}. \quad (4.52)$$

If the Lagrangian is hyperregular, the fibre derivative can be inverted in order to express v as a function $\eta(q, p)$. This in turn allows us to define the Hamiltonian,

$$H : T^*\mathcal{M} \rightarrow \mathbb{R}, \quad (4.53)$$

as the map

$$H : (q, p) \mapsto \langle p, \eta(q, p) \rangle - L(q, \eta(q, p)). \quad (4.54)$$

Thus, hyperregular Lagrangians on $T\mathcal{M}$ induce Hamiltonian systems on $T^*\mathcal{M}$. The transition from L on $T\mathcal{M}$ to H on $T^*\mathcal{M}$ is an example of the so called Legendre transform.

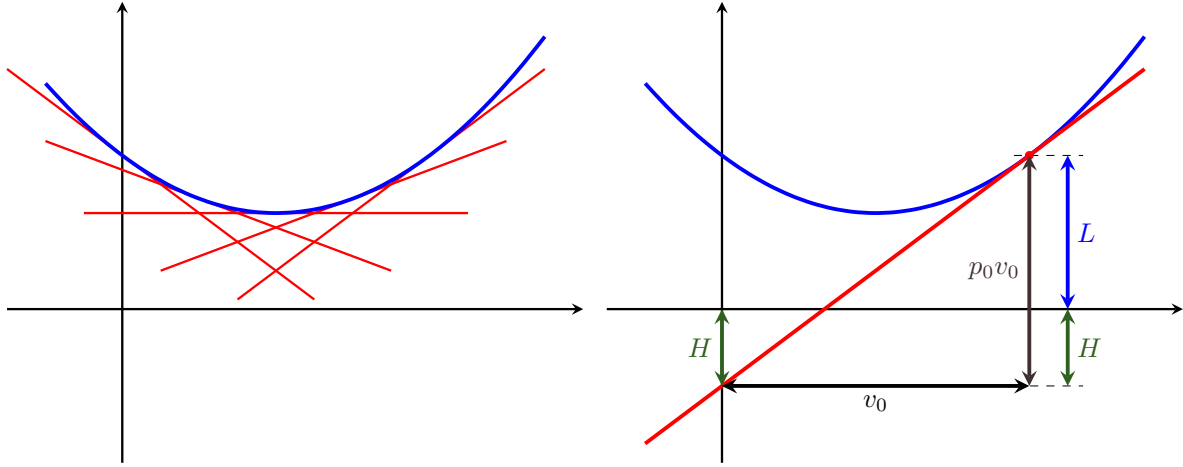


Fig. 4.2: Graphic representation of the Legendre transform $H(p)$ of $L(v)$. The blue curve is the graph of a convex function $L(v)$. The red lines are tangents to that function. On the right-hand side the tangent at $v = v_0$ has slope p_0 .

4.2.2 Geometry of the Legendre Transform

In this section, we want to explore the geometry behind the Legendre transform. We follow Arnold [3, Section 14], Jose and Saletan [41, section 5.1.2] and Zia, Redish, and McKay [81].

Consider a differentiable function $L(v)$ of a single variable v . Assume $L(v)$ to be convex, i.e., its second derivative d^2L/dv^2 is always positive. As a consequence, the slope function $p(v) = dL/dv$ is a monotonic function of v , so that there is a one-to-one mapping between v and the derivative dL/dv . Each slope occurs only at one point on the curve.

The Legendre transform provides a function $H(p)$ that contains the same information as $L(v)$ but as a function of p alone, with no reference to v . The function $H(p)$ is obtained in the following way. See Figure 4.2, which shows tangents to the graph of $L(v)$. If we pick one point v_0 , the slope of the corresponding tangent is $p(v_0) \equiv p_0$. Its intercept on the vertical axis is given by

$$I = L(v_0) - p_0 v_0. \quad (4.55)$$

For each v on the curve, there is a different intercept, so that the intercept is a function of the point v and the derivative p at that point,

$$I(v, p) = L(v) - pv. \quad (4.56)$$

As the function $p(v)$ is single-valued, it can be inverted to obtain v as a function of p . This function $v(p)$ is single-valued as well, so that each value of p uniquely determines a value of v . We can use the function $v(p)$ to replace v in (4.56), which then becomes a function of p alone. This defines the function $H(p)$,

$$H(p) \equiv -I(v(p), p) = pv(p) - L(v(p)). \quad (4.57)$$

Invertibility of $p(v)$ means that $p(v)$ does not pass through a minimum or maximum, i.e.,

$$\frac{dp}{dv} \neq 0. \quad (4.58)$$

As

$$\frac{dp}{dv} = \frac{d^2L}{dv^2}, \quad (4.59)$$

a necessary condition for invertibility is that the second derivative of L does never vanish, L must have no point of inflection. In higher dimensions, when $v = (v^1, v^2, \dots, v^n)$, the analytic treatment proceeds in complete analogy, even though the diagrammatic demonstration is much more difficult. The necessary condition for invertibility now becomes that the Hessian of L is non-singular,

$$\det \left| \frac{\partial^2 L}{\partial v^i \partial v^j} \right| \neq 0. \quad (4.60)$$

Here, we were considering functions L which only depend on the variable v for which we carry out the Legendre transform. For the Lagrangian this role is taken by the generalised velocities v . However, in addition, the Lagrangian also depends on generalised coordinates q . In that case, the Legendre transform is performed for each point in \mathcal{M} .

4.2.3 Hamilton Equations

The Euler-Lagrange equations (4.2) are equivalent to a system of ordinary differential equations, namely the Hamilton equations in canonical coordinates,

$$\dot{q}^i(t) = \frac{\partial H}{\partial p_i}(q(t), p(t)), \quad \dot{p}_i(t) = -\frac{\partial H}{\partial x^i}(q(t), p(t)), \quad i = 1, \dots, d, \quad (4.61)$$

where H is the Hamiltonian as defined in (4.54) and $(q(t), p(t))$ is a curve on the cotangent bundle $T^*\mathcal{M}$. It is easy to see that (4.61) and (4.29) are equivalent. With the definition of the generalised momentum (4.48) and the velocity v expressed as $\eta(q, p)$, we compute

$$\frac{\partial H}{\partial p_i} = \eta^i + p_j \frac{\partial \eta^j}{\partial p_i} - \frac{\partial L}{\partial v^j} \frac{\partial \eta^j}{\partial p_i} = \eta^i, \quad (4.62)$$

$$\frac{\partial H}{\partial x^i} = p^j \frac{\partial \eta^j}{\partial x^i} - \frac{\partial L}{\partial x^i} - \frac{\partial L}{\partial v^j} \frac{\partial \eta^j}{\partial x^i} = -\frac{\partial L}{\partial x^i}, \quad (4.63)$$

so that the first equation in (4.61) just becomes

$$\dot{q}^i(t) = \eta^i(q(t), p(t)), \quad (4.64)$$

and with (4.48) the second equation in (4.61) recovers the Euler-Lagrange equations,

$$\dot{p}_i(t) = -\frac{\partial H}{\partial x^i}(q(t), p(t)) \quad \leftrightarrow \quad \frac{d}{dt} \left(\frac{\partial L}{\partial v^i}(q(t), \dot{q}(t)) \right) = \frac{\partial L}{\partial x^i}(q(t), \dot{q}(t)). \quad (4.65)$$

Often, the Hamiltonian is given as the sum of kinetic energy T and potential energy U , where the kinetic energy is expressed in terms of momentum instead of velocity,

$$H(q, p) = T(p) + U(q), \quad (4.66)$$

and in particular,

$$H(q, p) = \frac{1}{2} p^T M^{-1} p + U(q). \quad (4.67)$$

That is, the Hamiltonian H corresponds to the total energy of the system. For systems where the Hamiltonian does not explicitly depend on time, H is an invariant, that is it is preserved by the dynamics of the system.

4.2.4 Symplectic Form

The Hamilton equations (4.61) can be combined into a single equation upon combining the dynamical variables q and p into a vector $z = (q, p)$ and introducing the symplectic matrix Ω , a skew-symmetric $2d \times 2d$ matrix,

$$\Omega = \begin{pmatrix} \mathbb{0}_{d \times d} & \mathbb{1}_{d \times d} \\ -\mathbb{1}_{d \times d} & \mathbb{0}_{d \times d} \end{pmatrix}. \quad (4.68)$$

Besides being skew-symmetric, the symplectic matrix Ω has the following properties,

$$\Omega^T = -\Omega, \quad \Omega^{-1} = -\Omega, \quad \Omega^2 = -\mathbb{1}. \quad (4.69)$$

With that, we can rewrite (4.61) as

$$\Omega^T \dot{z} = \nabla H(z) \quad \text{with} \quad \nabla = (\partial_x, \partial_p). \quad (4.70)$$

Definition 4.10. The **canonical symplectic form** ω is a differential two-form on $T^*\mathcal{M}$, defined by

$$\omega(V, W) = V^T \Omega W \quad \text{with} \quad V, W \in T(T^*\mathcal{M}). \quad (4.71)$$

On the cotangent bundle $T^*\mathcal{M}$, there exists a canonical one-form $\Theta \in \wedge^1(T^*\mathcal{M})$,

$$\Theta = \pi^* p, \quad (4.72)$$

where $\pi : T^*\mathcal{M} \rightarrow \mathcal{M}$ is the standard projection and $p = p_i dx^i$ is a one-form on \mathcal{M} . The symplectic form $\omega \in \wedge^2(T^*\mathcal{M})$ can be obtained from the canonical one-form Θ as

$$\omega = -d\Theta. \quad (4.73)$$

In local coordinates it is written

$$\omega = dx^i \wedge dp_i. \quad (4.74)$$

The pair $(T^*\mathcal{M}, \omega)$ is an example of a symplectic manifold.

4.2.5 Hamiltonian Vector Fields

Definition 4.11. Given a Hamiltonian H , the corresponding **Hamiltonian vector field** X_H is defined as the unique vector field on $T^*\mathcal{M}$ satisfying

$$\iota_{X_H} \omega = dH. \quad (4.75)$$

Writing the Hamiltonian vector field X_H in coordinates,

$$X_H = X_{x^i} \frac{\partial}{\partial x^i} + X_{p_i} \frac{\partial}{\partial p_i}, \quad (4.76)$$

or short $X_H = (X_x, X_p)$, we see that (4.75) is

$$-X_{p_i} dx^i + X_{x^i} dp_i = \frac{\partial H}{\partial x^i} dx^i + \frac{\partial H}{\partial p_i} dp_i, \quad (4.77)$$

so that in components, the Hamiltonian vector field X_H reads

$$X_H = \frac{\partial H}{\partial p_i} \frac{\partial}{\partial x^i} - \frac{\partial H}{\partial x^i} \frac{\partial}{\partial p_i}. \quad (4.78)$$

The Hamiltonian flow $F_H : T^*\mathcal{M} \times \mathbb{R} \rightarrow T^*\mathcal{M}$ is the flow of the Hamiltonian vector field X_H , that is the collection of maps $F_H^t : T^*\mathcal{M} \rightarrow T^*\mathcal{M}$ satisfying

$$\frac{d}{dt} F_H^t(z_0) = X_H(F_H^t(z_0)) \quad (4.79)$$

for each $z_0 \in T^*\mathcal{M}$ and $t \in \mathbb{R}$ and $F_H^0(z_0) = z_0$. Denoting by $z = (q, p)$ some path in the cotangent space $T^*\mathcal{M}$, the Hamilton equations (4.61) can be rewritten with respect to the Hamiltonian vector field X_H as

$$\frac{d}{dt} z(t) = X_H(z(t)). \quad (4.80)$$

Remark 4.12. *The Hamiltonian vector field X_H and flow map F_H are always well-defined for any Hamiltonian.*

4.2.6 Phasespace Action Principle

The Hamilton equations can also be derived from a variational principle on $T^*\mathcal{M}$. A curve (q, p) in $T^*\mathcal{M}$ satisfies the Hamilton equations (4.61) if and only if

$$\delta \int_{t_1}^{t_2} [\langle p(t), \dot{q}(t) \rangle - H(q(t), p(t))] dt = 0, \quad (4.81)$$

for variations over curves (q, p) in $T^*\mathcal{M}$ where $\dot{q} = dq/dt$ and where q is fixed at the endpoints but the variations of p are free. Computing the variations,

$$\int_{t_1}^{t_2} \left[\delta p_i \dot{q}^i + p_i \delta \dot{q}^i - \frac{\partial H}{\partial p_i}(q, p) \delta p_i - \frac{\partial H}{\partial x^i}(q, p) \delta q^i \right] dt = 0, \quad (4.82)$$

integrating by parts the second term and using $\delta q(t_1) = \delta q(t_2) = 0$,

$$\int_{t_1}^{t_2} \left[\left(\dot{q}^i - \frac{\partial H}{\partial p_i}(q, p) \right) \delta p_i - \left(\dot{p}_i + \frac{\partial H}{\partial x^i}(q, p) \right) \delta q^i \right] dt = 0, \quad (4.83)$$

we see that the variation vanishes for arbitrary δq^i and δp_i exactly when the Hamilton equations (4.61) hold.

4.2.7 Hamilton-Pontryagin Principle

The Hamilton-Pontryagin principle [67, 72, 79] is an action principle on the Pontryagin bundle $T\mathcal{M} \oplus T^*\mathcal{M}$. It is a very useful tool, e.g., for treating systems with constraints and degenerate Lagrangian systems, but also for constructing numerical integrators.

In Hamilton's principle of stationary action (4.30), the Lagrangian is evaluated at $(q(t), \dot{q}(t))$ that is the trajectories in $T\mathcal{M}$ are restricted to tangent lifts of trajectories q in \mathcal{M} and the variations

δv are induced by variations δx . In the Hamilton-Pontryagin principle, the variations of v are left free, but we add a kinematic constraint which ensures the second-order condition $v(t) = \dot{q}(t)$ with the momentum $p(t)$ as a Lagrange multiplier,

$$\delta \int \left[L(q, v) + \langle p, \dot{q} - v \rangle \right] dt = 0. \quad (4.84)$$

Computing variations,

$$\int \left[\frac{\partial L}{\partial x}(q, v) \delta q + \frac{\partial L}{\partial v}(q, v) \delta v + \langle \delta p, \dot{q} - v \rangle + \langle p, \delta \dot{q} - \delta v \rangle \right] dt = 0, \quad (4.85)$$

we find the second-order condition, the Legendre transform, and the Euler-Lagrange equations,

$$\dot{q} = v, \quad p = \frac{\partial L}{\partial v}(q, v), \quad \dot{p} = -\frac{\partial L}{\partial x}(q, v). \quad (4.86)$$

These equations describe the evolution of a curve $t \mapsto (q(t), v(t), p(t))$ on the Pontryagin bundle $T\mathcal{M} \oplus T^*\mathcal{M}$. For constrained systems, the Hamilton-Pontryagin principle is generalised to the Lagrange–d'Alembert–Pontryagin principle and the Hamilton–d'Alembert principle in phasespace [79].

4.3 Symplecticity

Consider the canonical symplectic form (4.71) for the simple case when $d = 1$ and $\mathcal{M} = \mathbb{R}$ so that $T^*\mathcal{M} \cong \mathbb{R}^2$, and define two tangent vectors on the cotangent bundle $T^*\mathcal{M}$,

$$V = V^x \frac{\partial}{\partial x} + V^p \frac{\partial}{\partial p}, \quad W = W^x \frac{\partial}{\partial x} + W^p \frac{\partial}{\partial p}, \quad V, W \in T(T^*\mathcal{M}). \quad (4.87)$$

In that case, $\omega(V, W)$ corresponds to the oriented area of the parallelogram P spanned by V and W ,

$$\omega(V, W) = \det \begin{pmatrix} V^x & W^x \\ V^p & W^p \end{pmatrix} = V^x W^p - V^p W^x. \quad (4.88)$$

In higher dimensions, this is replaced with the sum of oriented areas of the projections of P onto the coordinate planes (x^i, p^i) , i.e.,

$$\omega(V, W) = \sum_{i=1}^d \det \begin{pmatrix} V^{x^i} & W^{x^i} \\ V^{p_i} & W^{p_i} \end{pmatrix} = \sum_{i=1}^d V^{x^i} W^{p_i} - V^{p_i} W^{x^i}. \quad (4.89)$$

As a two-form, ω defines a bilinear map acting on a pair of vectors from $T(T^*\mathcal{M})$, which plays a central role in Hamiltonian systems.

4.3.1 Symplectic Maps

A linear map $A : T^*\mathcal{M} \rightarrow T^*\mathcal{M}$ is called symplectic if

$$A^T \Omega A = \Omega \quad \text{or} \quad \omega(A_* V, A_* W) = \omega(V, W). \quad (4.90)$$

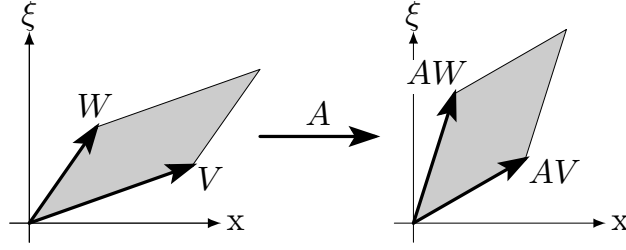


Fig. 4.3: Symplecticity of a linear map A .

For $d = 1$, symplecticity of a linear mapping A therefore corresponds to area preservation of A . For $d > 1$, symplecticity means that the sum of the projections of the parallelogram P onto the (x^i, p^i) planes are the same as for the mapped parallelogram $A(P)$.

Most often, we deal with nonlinear mappings. As those are usually differentiable functions, they can locally be approximated by linear mappings. Therefore a differentiable map $\varphi : T^*\mathcal{M} \rightarrow T^*\mathcal{M}$ is called symplectic if the Jacobian $\varphi'(x, p)$ is everywhere symplectic, i.e.,

$$\varphi'(x, p)^T \Omega \varphi'(x, p) = \Omega \quad \text{for all } (x, p) \in T^*\mathcal{M}, \quad (4.91)$$

or equivalently

$$\omega(\varphi'(x, p)V, \varphi'(x, p)W) = \omega(V, W), \quad (4.92)$$

or

$$\omega(\varphi_*V, \varphi_*W) = \omega(V, W), \quad (4.93)$$

or

$$\varphi^*\omega(V, W) = \omega(V, W), \quad (4.94)$$

for all $(x, p) \in T^*\mathcal{M}$ with $V, W \in T_{(x,p)}(T^*\mathcal{M})$. We can now show that the flow of a Hamiltonian system is a symplectic map.

4.3.2 Hamiltonian Flows Preserve the Symplectic Form

Denote coordinates on the cotangent bundle $T^*\mathcal{M}$ by $z = (x, p)$ and a path on $T^*\mathcal{M}$ by $z = (q, p)$. Given a Hamiltonian $H : T^*\mathcal{M} \rightarrow \mathbb{R}$, the corresponding Hamiltonian vector field X_H is defined by

$$X_H(z) = \Omega \nabla H(z). \quad (4.95)$$

It is the dynamical vector field on $T^*\mathcal{M}$ that solves the Hamilton equations (4.61). The corresponding flow map

$$F_H^t : T^*\mathcal{M} \rightarrow T^*\mathcal{M}, \quad (4.96)$$

is the mapping that advances the solution by time t , i.e.,

$$F_H^t : z(0) \mapsto z(t). \quad (4.97)$$

It takes initial values $z_0 = z(0) = (q(0), p(0))$ to points $z(t)$ of the corresponding phasespace trajectory at time t , hence $z(t) = F_H^t(z_0)$ and

$$\frac{d}{dt}F_H^t(z_0) = \dot{z}(t) = \Omega \nabla H(z(t)) = \Omega \nabla H(F_H^t(z_0)). \quad (4.98)$$

The relation between the Hamiltonian flow and its vector field is given by

$$X_H(z_0) = \left. \frac{d}{dt} F_H^t(z_0) \right|_{t=0} \quad \text{for all } z_0 \in T^*\mathcal{M}. \quad (4.99)$$

The Hamiltonian flow F_H^t of the Hamiltonian vector field X_H preserves the symplectic form ω ,

$$\mathcal{L}_{X_H} \omega = 0. \quad (4.100)$$

Using Cartan's magic formula (infinitesimal homotopy relation), the Lie derivative becomes

$$\mathcal{L}_{X_H} \omega = d(\iota_{X_H} \omega) + \iota_{X_H} (d\omega) = 0. \quad (4.101)$$

As the symplectic two-form is exact, $\omega = -d\Theta$, and therefore closed, we immediately see that the second term on the right-hand side vanishes. Moreover, $\iota_{X_H} \omega = dH$, so that the first term is also seen to vanish. This proof is short and elegant, but it does not immediately translate to the discrete setting. Therefore we will consider an alternative strategy in the following.

Theorem 4.13. *Let $H(z)$ be a twice continuously differentiable function on $T^*\mathcal{M}$ with Hamiltonian vector field X_H . For each fixed t , the corresponding Hamiltonian flow F_H^t is a symplectic transformation.*

Proof. Define

$$\Psi(t) = \frac{dF_H^t}{d\zeta}(z_0), \quad (4.102)$$

which solves the (first) variational equation

$$\dot{\Psi}(t) = \Omega \nabla^2 H(F_H^t(z_0)) \Psi(t), \quad (4.103)$$

as can be seen by applying the chain rule to (4.98),

$$\begin{aligned} \dot{\Psi}(t) &= \frac{\partial}{\partial t} \left(\frac{\partial}{\partial \zeta} F_H^t(z_0) \right) \\ &= \frac{\partial}{\partial \zeta} \left(\frac{\partial}{\partial t} F_H^t(z_0) \right) \\ &= \frac{\partial}{\partial \zeta} \left(\Omega \nabla H(F_H^t(z_0)) \right) \\ &= \Omega \nabla^2 H(F_H^t(z_0)) \frac{\partial F_H^t}{\partial \zeta}(z_0), \end{aligned} \quad (4.104)$$

where $\nabla^2 H(z)$ is the Hessian of $H(z)$, that is a symmetric $2d \times 2d$ matrix. We therefore obtain

$$\begin{aligned} \frac{d}{dt} \left((F_H^t)'^T \Omega (F_H^t)' \right) &= \left(\Omega \nabla^2 H(F_H^t) \Psi \right)^T \Omega \Psi + \Psi^T \Omega \left(\Omega \nabla^2 H(F_H^t) \Psi \right) \\ &= \Psi^T \nabla^2 H(F_H^t)^T \Omega^T \Omega \Psi + \Psi^T \Omega \Omega \nabla^2 H(F_H^t) \Psi = 0. \end{aligned} \quad (4.105)$$

As $\nabla^2 H$ is symmetric, $\Omega^2 = -\mathbb{1}$ and $\Omega^T \Omega = \mathbb{1}$, this expression vanishes. Further, as F_H^0 is the identity map, the relation

$$(F_H^t)'^T \Omega (F_H^t)' = \Omega \quad (4.106)$$

is satisfied for $t = 0$ and therefore it is satisfied for all t and all $z_0 = (q_0, p_0)$. \square

Symplecticity is a characteristic property of Hamiltonian systems. However, the symplectic form can also be obtained in the Lagrangian formalism without any reference to the Hamiltonian formalism.

4.3.3 Variational Route to the Cartan Form

In this section we want to describe a variational derivation of the Cartan form. Its exterior derivative is the symplectic form and together these are the two fundamental geometric structures of classical mechanics. In most treatments, the Cartan form and the symplectic form are constructed by using the Legendre transformation to pull back the canonical forms from the Hamiltonian side (cotangent bundle) to the Lagrangian side (tangent bundle). However, the Cartan form arises naturally in the boundary term of the variation of the action in Hamilton's action principle, thus allowing to obtain these structures while staying on the Lagrangian side entirely, without any reference to the Hamiltonian side. The advantage of this approach is the possibility of a geometric treatment of theories for which a Hamiltonian cannot be defined.

Besides leading to the equations of motion, the variational principle provides a direct and natural way to derive the fundamental geometric structures of classical mechanics. For this derivation, the boundary conditions $\delta q(t_1) = \delta q(t_2) = 0$ are removed, while the time interval is kept fixed. Thus the variational principle reads

$$\delta \mathcal{A}[q] = d\mathcal{A}[q] \cdot \delta q = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial x}(q(t), \dot{q}(t)) - \frac{d}{dt} \frac{\partial L}{\partial v}(q(t), \dot{q}(t)) \right] \cdot \delta q(t) dt + \left[\frac{\partial L}{\partial v}(q(t), \dot{q}(t)) \cdot \delta q(t) \right]_{t_1}^{t_2} \quad (4.107)$$

where the variations δq do not vanish at the boundary point, so that the last term on the right hand side does not vanish. This last term corresponds to a linear pairing of the function $\partial L / \partial v$, which is a function of (q, \dot{q}) , with the tangent vector δq . This term can be regarded as a one-form on $T\mathcal{M}$, referred to as the Lagrangian one-form or Cartan one-form,

$$\Theta_L = \frac{\partial L}{\partial v} dx. \quad (4.108)$$

One could be tempted to regard $\partial L / \partial v$ as a one-form on \mathcal{M} as it only has a component in dx . The same way δq could be regarded as a tangent vector on \mathcal{M} . However, $\partial L / \partial v$ is a function of (q, \dot{q}) and therefore clearly a function on $T\mathcal{M}$. δq can also be replaced with a more general vector $\delta \hat{q} \in T(T\mathcal{M})$ that has non-vanishing components $(\delta x, \delta v)$.

The Lagrangian one-form Θ_L is the boundary term of the functional derivative of the action, if the boundary is varied. The negative of the exterior derivative of the Lagrangian one-form gives the Lagrangian two-form, also referred to as the symplectic two-form

$$\omega_L \equiv -d\Theta_L, \quad (4.109)$$

given in coordinates by

$$\omega_L = \frac{\partial^2 L}{\partial x^i \partial v^j} dx^i \wedge dx^j + \frac{\partial^2 L}{\partial v^i \partial v^j} dv^i \wedge dx^j. \quad (4.110)$$

For details on the connection between the Lagrangian one-form Θ_L on $T\mathcal{M}$ and the canonical one-form Θ on $T^*\mathcal{M}$ as well as between the Lagrangian two-form ω_L on $T\mathcal{M}$ and the canonical symplectic two-form ω on $T^*\mathcal{M}$ the reader is referred to Marsden and Ratiu [54].

4.3.4 Lagrangian Flows Preserve the Symplectic Form

Denote the vector field on $\mathcal{T}\mathcal{M}$ that solves the Euler-Lagrange equations by X_L . Its flow F_L^t , referred to as the Lagrangian flow, is a map

$$F_L^t : \mathcal{T}\mathcal{M} \rightarrow \mathcal{T}\mathcal{M}, \quad (4.111)$$

taking initial values (q_0, \dot{q}_0) to points of the corresponding phasespace trajectory at time t , that is

$$F_L^t : (q_0, \dot{q}_0) \mapsto (q(t), \dot{q}(t)), \quad (4.112)$$

such that

$$\frac{\partial L}{\partial x}((q(t), \dot{q}(t))) - \frac{d}{dt} \frac{\partial L}{\partial v}((q(t), \dot{q}(t))) = 0. \quad (4.113)$$

The Lagrangian vector field is accordingly defined as

$$X_L(q_0, \dot{q}_0) = \left. \frac{d}{dt} F_L^t(q_0, \dot{q}_0) \right|_{t=0}. \quad (4.114)$$

Restrict the action \mathcal{A} to the subspace $\mathcal{Q}_L \subset \mathcal{Q}(\mathcal{M})$ of solutions of the Euler-Lagrange equations. Elements $q \in \mathcal{Q}_L$ are integral curves of X_L , and therefore uniquely determined by the initial condition $v_q = (q(0), \dot{q}(0)) \in \mathcal{T}\mathcal{M}$. Consequently, \mathcal{Q}_L may be identified with the space of initial conditions, i.e., \mathcal{Q}_L is isomorphic to $\mathcal{T}\mathcal{M}$.

Associate to v_q the integral curve $t \mapsto F_L^t(v_q)$ with $t \in [t_1, t_2]$

$$q(t) = \pi_{\mathcal{Q}}(F_L^t(v_q)) \quad \text{with} \quad F_L^t(v_q) = (q(t), \dot{q}(t)). \quad (4.115)$$

The restricted action \mathcal{A}_t corresponds to the value of \mathcal{A} on that curve. It defines a map

$$\mathcal{A}_t : \mathcal{T}\mathcal{M} \rightarrow \mathbb{R} \quad (4.116)$$

by

$$\mathcal{A}_t[v_q] = \mathcal{A}[q] \quad \text{with} \quad q \in \mathcal{Q}_L \quad \text{and} \quad (q(0), \dot{q}(0)) = v_q. \quad (4.117)$$

or explicitly

$$\mathcal{A}_t[v_q] = \int_{t_1}^{t_2} L(q(t), \dot{q}(t)) dt = \int_{t_1}^{t_2} L(F_L^t(v_q)) dt \quad (4.118)$$

Calculating the variation of the restricted action,

$$d\mathcal{A}[q] \cdot \delta q = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial x}(q, \dot{q}) - \frac{d}{dt} \left(\frac{\partial L}{\partial v}(q, \dot{q}) \right) \right] \cdot \delta \hat{q} dt + \left[\frac{\partial L}{\partial v}(q, \dot{q}) \cdot \delta \hat{q} \right]_{t_1}^{t_2}. \quad (4.119)$$

the first term on the right-hand side vanishes (see also (4.37)), as \mathcal{A} is restricted to solutions of the Euler-Lagrange equations,

$$d\mathcal{A}[q] \cdot \delta q = \left[\frac{\partial L}{\partial v}(q, \dot{q}) \cdot \delta \hat{q} \right]_0^t \quad \text{with} \quad q \in \mathcal{Q}_L. \quad (4.120)$$

As \mathcal{A}_t is considered a real-valued function on $\mathbb{T}Q$, this becomes

$$d\mathcal{A}_t[v_q] \cdot w_{v_q} = \Theta_L(F_L^t(v_q)) \cdot \frac{d}{d\epsilon} F_L^t(v_q^\epsilon) \Big|_{\epsilon=0} - \Theta_L(v_q) \cdot w_{v_q} \quad (4.121)$$

with v_q^ϵ an arbitrary curve in $\mathbb{T}M$, namely

$$v_q^\epsilon : \mathbb{R} \rightarrow \mathbb{T}M \quad \text{such that} \quad v_q^0 = v_q \quad \text{and} \quad w_{v_q} = \frac{d}{d\epsilon} v_q^\epsilon \Big|_{\epsilon=0}. \quad (4.122)$$

Since w_{v_q} is arbitrary, (4.121) is equivalent to

$$d\mathcal{A}_t = (F_L^t)^* \Theta_L - \Theta_L. \quad (4.123)$$

Taking the exterior derivative

$$0 = d^2 \mathcal{A}_t = d((F_L^t)^* \Theta_L - \Theta_L) = -(F_L^t)^* \omega_L + \omega_L. \quad (4.124)$$

leads to the conservation of the symplectic form ω_L along the Lagrangian flow X_L

$$(F_L^t)^* \omega_L = \omega_L. \quad (4.125)$$

These results can be considered the Lagrangian equivalent of the well-known conservation of the symplectic form by Hamiltonian flows (c.f. section 4.3.2).

4.4 Noether Theorem

The Noether theorem [63, 43, 62] is one of the deepest and most influential insights of mathematical physics. It states that each continuous symmetry of a Lagrangian corresponds to a conservation law of the associated Euler-Lagrange equations and vice versa.

4.4.1 One-Parameter Groups of Transformations

Consider infinitesimal transformation

$$q(t) \rightarrow q^\epsilon(t) = \sigma(t, q(t), \epsilon) = \sigma^\epsilon(t, q(t)) \quad \text{with} \quad \sigma^0 = \text{id}, \quad (4.126)$$

such that

$$\dot{q}^\epsilon(t) = \frac{d}{dt} q^\epsilon(t), \quad q^0(t) = q(t), \quad \dot{q}^0(t) = \dot{q}(t). \quad (4.127)$$

We have a symmetry if the Lagrangian is invariant under this transformation

$$L(q^\epsilon(t), \dot{q}^\epsilon(t)) = L(q(t), \dot{q}(t)), \quad (4.128)$$

or equivalently

$$\frac{d}{d\epsilon} \Big|_{\epsilon=0} L(q^\epsilon(t), \dot{q}^\epsilon(t)) = 0. \quad (4.129)$$

Computing this explicitly, we find

$$\left. \frac{d}{d\epsilon} \right|_{\epsilon=0} L(q^\epsilon, \dot{q}^\epsilon) = \left. \frac{\partial L}{\partial \mathbf{x}}(q, \dot{q}) \cdot \frac{d\sigma^\epsilon}{d\epsilon} \right|_{\epsilon=0} + \left. \frac{\partial L}{\partial \mathbf{v}}(q, \dot{q}) \cdot \frac{d\dot{\sigma}^\epsilon}{d\epsilon} \right|_{\epsilon=0} \quad (4.130)$$

$$= \frac{\partial L}{\partial \mathbf{x}}(q, \dot{q}) \cdot X + \frac{\partial L}{\partial \mathbf{v}}(q, \dot{q}) \cdot \dot{X} = 0, \quad (4.131)$$

with the generating vector field

$$X = \left. \frac{d\sigma^\epsilon}{d\epsilon} \right|_{\epsilon=0}. \quad (4.132)$$

If $q(t)$ solves the Euler-Lagrange equations, we can replace the first term on the right-hand side

$$\left[\frac{d}{dt} \frac{\partial L}{\partial \mathbf{v}}(q, \dot{q}) \right] \cdot X + \frac{\partial L}{\partial \mathbf{v}}(q, \dot{q}) \cdot \left[\frac{d}{dt} X \right] = 0. \quad (4.133)$$

This is a total time derivative which constitutes a conservation law corresponding to a symmetry of the Lagrangian generated by X for solutions q of the Euler-Lagrange equations. In short, we can write

$$\frac{d}{dt} \left[\frac{\partial L}{\partial \mathbf{v}}(q, \dot{q}) \cdot X \right] = 0, \quad X = \left. \frac{d\sigma^\epsilon}{d\epsilon} \right|_{\epsilon=0}, \quad (4.134)$$

which states that the momentum $p = \partial L / \partial \mathbf{v}(q, \dot{q})$ is conserved in the direction of X .

Example 4.14 (Example: Point Particle). *Consider a simple transformation that amounts to a time-independent translation*

$$q^\epsilon(t) = q(t) + \epsilon X, \quad \dot{q}^\epsilon(t) = \dot{q}(t). \quad (4.135)$$

The corresponding transformed Lagrangian is

$$L(q^\epsilon(t), \dot{q}^\epsilon(t)) = \frac{m}{2} (\dot{q}(t))^2 = L(q, \dot{q}) \quad (4.136)$$

which is obviously the same as the untransformed Lagrangian. The symmetry condition is therefore trivially fulfilled

$$\left. \frac{\partial}{\partial \epsilon} \right|_{\epsilon=0} L(q^\epsilon(t), \dot{q}^\epsilon(t)) = 0 \quad (4.137)$$

and the corresponding conservation law

$$\frac{d}{dt} \left[\frac{\partial L}{\partial \mathbf{v}}(q, \dot{q}) \cdot X \right] = \frac{d}{dt} [m\dot{q} \cdot X] = 0 \quad (4.138)$$

states that momentum is preserved in direction of X .

5 Symplectic Integrators

A numerical integrator φ_t is a mapping which approximates the flow map ϕ_t of a given system of differential equations. Many standard methods are constructed in order to minimise the local error of the numerical solution, that is the difference between the numerical solution and the exact solution during one solution step. This often leads to numerical solutions, which gradually drift away from the exact solution as errors are accumulated in each time step. In the construction of geometric integrators, structural properties of the flow map are imposed on the numerical integrator, which leads to improved behaviour in simulations. With geometric integrators error accumulation e.g. in the energy of the system is usually absent, so that even for very long integration times a good qualitative agreement between the numerical and the exact solutions is observed.

The first class of such geometric integrators we want to study are symplectic integrators. The solution of a Hamiltonian system is a symplectic transformation, that is an area preserving map. The numerical solution obtained by traditional integrators is in general not a symplectic transformation and therefore will be spuriously damped or excited. The numerical solution obtained by a symplectic integrator is a symplectic transformation, therefore showing dramatically improved long-time behaviour.

Definition 5.1. *A numerical one-step method is called **symplectic** if the numerical flow*

$$z_{n+1} = \varphi_h(z_n), \quad z_n = (q_n, p_n)^T, \quad (5.1)$$

is symplectic, i.e.,

$$(\varphi'_h)^T \Omega (\varphi'_h) = \Omega, \quad (5.2)$$

or equivalently

$$dq_{n+1} \wedge dp_{n+1} = dq_n \wedge dp_n, \quad (5.3)$$

whenever the method is applied to a smooth canonical Hamiltonian system.

The field of symplectic integration has received a lot of attention since the pioneering work of de Vogelaere [19] and is by now very well developed. Several books discuss the topic, namely Sanz-Serna and Calvo [70], Leimkuhler and Reich [48], Hairer, Lubich, and Wanner [31], Feng and Qin [23] and Blanes and Casas [7].

5.1 Symplectic Euler

The simplest symplectic integrators are the *symplectic Euler methods*, Euler-A,

$$q_{n+1} = q_n + h H_p(q_{n+1}, p_n) \quad (\text{implicit Euler for } q), \quad (5.4a)$$

$$p_{n+1} = p_n - h H_x(q_{n+1}, p_n) \quad (\text{explicit Euler for } p). \quad (5.4b)$$

and Euler-B,

$$p_{n+1} = p_n - h H_x(q_n, p_{n+1}) \quad (\text{implicit Euler for } p), \quad (5.5a)$$

$$q_{n+1} = q_n + h H_p(q_n, p_{n+1}) \quad (\text{explicit Euler for } q), \quad (5.5b)$$

These are symplectic methods of order 1, where the order follows from standard arguments, e.g., Taylor expansion. In case of a separable Hamiltonian $H(p, q) = T(p) + U(q)$, both methods are explicit. The symplectic Euler methods are mutually adjoint.

Definition 5.2. The method φ_h^* defined by

$$\varphi_h^* = \varphi_{-h}^{-1}, \quad (5.6)$$

is called the **adjoint method** of φ_h .

Given a method φ_h , its adjoint method φ_h^* is implicitly defined by

$$\varphi_h^* \circ \varphi_{-h} = \text{id}. \quad (5.7)$$

Exercise. Verify that the symplectic Euler methods are mutually adjoint.

Solution.

Compute the numerical flow of Euler-A,

$$\begin{pmatrix} \bar{q} \\ \bar{p} \end{pmatrix} = \varphi_h \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} q \\ p \end{pmatrix} + h \begin{pmatrix} +\partial_p H(\bar{q}, p) \\ -\partial_x H(\bar{q}, p) \end{pmatrix},$$

as well as the numerical flow of Euler-B,

$$\begin{pmatrix} \bar{q} \\ \bar{p} \end{pmatrix} = \varphi_h^* \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} q \\ p \end{pmatrix} + h \begin{pmatrix} +\partial_p H(q, \bar{p}) \\ -\partial_x H(q, \bar{p}) \end{pmatrix}.$$

Upon computing φ_h^{-1} ,

$$\begin{pmatrix} q \\ p \end{pmatrix} = \varphi_h^{-1} \begin{pmatrix} \bar{q} \\ \bar{p} \end{pmatrix} = \begin{pmatrix} \bar{q} \\ \bar{p} \end{pmatrix} - h \begin{pmatrix} +\partial_p H(\bar{q}, p) \\ -\partial_x H(\bar{q}, p) \end{pmatrix} = \varphi_{-h}^* \begin{pmatrix} \bar{q} \\ \bar{p} \end{pmatrix},$$

we find $\varphi_h^{-1} = \varphi_{-h}^*$, which is the condition for φ_h and φ_h^* to be mutually adjoint.

5.1.1 Symplecticity

In order to proof symplecticity of the Euler methods, we rewrite both methods in the form

$$f(z_n, z_{n+1}) = 0, \quad (5.8)$$

with

$$z_n = \begin{pmatrix} q_n \\ p_n \end{pmatrix}, \quad f(z_n, z_{n+1}) = \begin{pmatrix} f^q(z_n, z_{n+1}) \\ f^p(z_n, z_{n+1}) \end{pmatrix}. \quad (5.9)$$

For the Euler-B method, we have

$$f(z_n, z_{n+1}) = \begin{pmatrix} q_{n+1} - q_n - h H_p(q_n, p_{n+1}) \\ p_{n+1} - p_n + h H_x(q_n, p_{n+1}) \end{pmatrix}. \quad (5.10a)$$

We use the implicit function theorem,

$$\left(\frac{\partial f}{\partial z_{n+1}} \right) \left(\frac{\partial z_{n+1}}{\partial z_n} \right) + \left(\frac{\partial f}{\partial z_n} \right) = 0, \quad (5.11)$$

to compute φ'_h ,

$$\varphi'_h = \left(\frac{\partial z_{n+1}}{\partial z_n} \right) = - \left(\frac{\partial f}{\partial z_{n+1}} \right)^{-1} \left(\frac{\partial f}{\partial z_n} \right), \quad (5.12)$$

so that

$$\varphi'_h = \begin{pmatrix} \mathbb{1} & -hH_{pp} \\ 0 & \mathbb{1} + hH_{xp} \end{pmatrix}^{-1} \begin{pmatrix} \mathbb{1} + hH_{px} & 0 \\ -hH_{xx} & \mathbb{1} \end{pmatrix}. \quad (5.13)$$

Using the following formula for the inverse of a 2×2 block matrix,

$$M^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix} \quad \text{for} \quad M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad (5.14)$$

we obtain

$$\varphi'_h = \begin{pmatrix} \mathbb{1} & hH_{pp}(\mathbb{1} + hH_{xp})^{-1} \\ 0 & (\mathbb{1} + hH_{xp})^{-1} \end{pmatrix} \begin{pmatrix} \mathbb{1} + hH_{px} & 0 \\ -hH_{xx} & \mathbb{1} \end{pmatrix}.$$

Upon setting $A = \mathbb{1} + hH_{xp}$, this becomes

$$\varphi'_h = \begin{pmatrix} \mathbb{1} + hH_{xp}^T - h^2H_{pp}A^{-1}H_{xx} & hH_{pp}A^{-1} \\ -hA^{-1}H_{xx} & A^{-1} \end{pmatrix}. \quad (5.15)$$

After some algebra, namely

$$\begin{aligned} & \begin{pmatrix} A^{-1} & -hA^{-1}H_{qq} \\ hH_{pp}A^{-1} & \mathbb{1} + hH_{xp}^T - h^2H_{pp}A^{-1}H_{xx} \end{pmatrix}^T \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} A^{-1} & -hA^{-1}H_{qq} \\ hH_{pp}A^{-1} & \mathbb{1} + hH_{xp}^T - h^2H_{pp}A^{-1}H_{xx} \end{pmatrix} \\ &= \begin{pmatrix} A^{-T} & hA^{-T}H_{pp} \\ -hH_{xx}A^{-T} & A - h^2H_{xx}A^{-T}H_{pp} \end{pmatrix} \begin{pmatrix} hH_{pp}A^{-1} & A^T - h^2H_{pp}A^{-1}H_{xx} \\ -A^{-1} & hA^{-1}H_{xx} \end{pmatrix} \\ &= \begin{pmatrix} hA^{-T}H_{pp}A^{-1} - hA^{-T}H_{pp}A^{-1} & \\ -h^2H_{xx}A^{-T}H_{pp}A^{-1} - AA^{-1} + h^2H_{xx}A^{-T}H_{pp}A^{-1} & \\ & A^{-T}A^T - h^2A^{-T}H_{pp}A^{-1}H_{xx} + h^2A^{-T}H_{pp}A^{-1}H_{xx} \\ & -hH_{xx}A^{-T}A^T + h^3H_{xx}A^{-T}H_{pp}A^{-1}H_{xx} + hAA^{-1}H_{xx} - h^3H_{xx}A^{-T}H_{pp}A^{-1}H_{xx} \end{pmatrix} \\ &= \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}, \end{aligned}$$

we indeed find that

$$(\varphi'_h)^T \Omega (\varphi'_h) = \Omega. \quad (5.16)$$

Alternatively to the matrix-based approach, we can also show symplecticity by a differential approach. Compute the exterior derivative of the first symplectic Euler method,

$$dq_{n+1} = dq_n + h H_{px}(q_n, p_{n+1}) dq_n + h H_{pp}(q_n, p_{n+1}) dp_{n+1}, \quad (5.17a)$$

$$dp_{n+1} = dp_n - h H_{xx}(q_n, p_{n+1}) dq_n - h H_{xp}(q_n, p_{n+1}) dp_{n+1}. \quad (5.17b)$$

This implicit system of linear equations can be thought of as the discrete variational equations associated with (5.5). Take the wedge product of the first equation with dp_{n+1} and wedge product of dq_n with the second equation,

$$dq_{n+1} \wedge dp_{n+1} = dq_n \wedge dp_{n+1} + h H_{px}(q_n, p_{n+1}) dq_n \wedge dp_{n+1}, \quad (5.18a)$$

$$dq_n \wedge dp_{n+1} = dq_n \wedge dp_n - h dq_n \wedge H_{xp}(q_n, p_{n+1}) dp_{n+1}. \quad (5.18b)$$

Inserting the second expression into the first, we find that

$$dq_{n+1} \wedge dp_{n+1} = dq_n \wedge dp_n. \quad (5.19)$$

The proofs for the second method follow along the same lines.

5.2 Störmer-Verlet

The Störmer-Verlet methods (see Hairer, Lubich, and Wanner [32])

$$p_{n+1/2} = p_n - \frac{h}{2} H_x(q_n, p_{n+1/2}), \quad (5.20a)$$

$$q_{n+1} = q_n + \frac{h}{2} [H_p(q_n, p_{n+1/2}) + H_p(q_{n+1}, p_{n+1/2})], \quad (5.20b)$$

$$p_{n+1} = p_{n+1/2} - \frac{h}{2} H_x(q_{n+1}, p_{n+1/2}), \quad (5.20c)$$

and

$$q_{n+1/2} = q_n + \frac{h}{2} H_p(q_{n+1/2}, p_n), \quad (5.21a)$$

$$p_{n+1} = p_n - \frac{h}{2} [H_x(q_{n+1/2}, p_n) + H_x(q_{n+1/2}, p_{n+1})], \quad (5.21b)$$

$$q_{n+1} = q_{n+1/2} + \frac{h}{2} H_p(q_{n+1/2}, p_{n+1}), \quad (5.21c)$$

are symmetric, symplectic methods of order 2, explicit for separable Hamiltonians. Symplecticity follows immediately as the Störmer-Verlet methods are compositions of the two symplectic Euler methods $\varphi_{h/2}^A \circ \varphi_{h/2}^B$ and $\varphi_{h/2}^B \circ \varphi_{h/2}^A$, respectively, and the composition of symplectic maps is itself a symplectic map. This becomes evident if we split the second step of e.g. (5.20) into

$$q_{n+1/2} = q_n + \frac{h}{2} H_p(q_n, p_{n+1/2}), \quad (5.22a)$$

$$q_{n+1} = q_{n+1/2} + \frac{h}{2} H_p(q_{n+1}, p_{n+1/2}). \quad (5.22b)$$

For separable Hamiltonians, a second way of proving symplecticity is by interpreting the Störmer-Verlet methods as splitting methods. A third way of proving symplecticity is by showing that the Störmer-Verlet methods follow from a discrete action principle. As the composition of a method with its adjoint is always symmetric, the fact that the Störmer-Verlet methods are compositions of the two symplectic Euler methods immediately proves that the Störmer-Verlet methods are symmetric. Order 2 follows as symmetric methods always have even order.

Definition 5.3. A method φ_h is called symmetric if $\varphi_h = \varphi_h^*$ and therefore $\varphi_h^{-1} = \varphi_{-h}$.

5.3 Splitting Methods

Splitting is a simple technique which often leads to well-working symplectic integrators. Suppose that the Hamiltonian H can be split into the sum of $k \geq 2$ Hamiltonians H_i with $1 \leq i \leq k$, i.e.,

$$H(z) = \sum_{i=1}^k H_i(z), \quad (5.23)$$

with each Hamiltonian vector field

$$\dot{z} = \Omega^{-T} \nabla H_i(z) \quad (5.24)$$

explicitly solvable. The exact solution $\phi_t^{H_i}$ of each subsystem provides a symplectic map. As the composition of symplectic maps yields a symplectic map, a symplectic integrator can be obtained by an appropriate composition of the flow maps of each subsystem. A first-order symplectic integrator is obtained from the Lie-Trotter splitting,

$$\varphi_h = \phi_h^{H_1} \circ \phi_h^{H_2} \circ \dots \circ \phi_h^{H_k}. \quad (5.25)$$

Second-order symplectic integrators are obtained from symmetric splittings,

$$\varphi_h = \phi_{h/2}^{H_1} \circ \phi_{h/2}^{H_2} \circ \dots \circ \phi_{h/2}^{H_{k-1}} \circ \phi_h^{H_k} \circ \phi_{h/2}^{H_{k-1}} \circ \dots \circ \phi_{h/2}^{H_2} \circ \phi_{h/2}^{H_1}, \quad (5.26)$$

or

$$\varphi_h = \phi_{h/2}^{H_k} \circ \phi_{h/2}^{H_{k-1}} \circ \dots \circ \phi_{h/2}^{H_2} \circ \phi_h^{H_1} \circ \phi_{h/2}^{H_2} \circ \dots \circ \phi_{h/2}^{H_{k-1}} \circ \phi_{h/2}^{H_k}. \quad (5.27)$$

Higher order integrators can be constructed by using the Baker-Campbell-Hausdorff formula.

5.3.1 Separable Hamiltonian Systems

If we have a Hamiltonian of the form $H(p, q) = T(p) + U(q)$, we can consider only the subsystem with Hamiltonian $U(q)$,

$$\dot{q} = 0, \quad \dot{p} = -\nabla U(q). \quad (5.28)$$

This system can be solved exactly. The exact flow is

$$\phi_t^U(q, p) = \begin{pmatrix} q \\ p - t \nabla U(q) \end{pmatrix}. \quad (5.29)$$

Next, consider the subsystem with Hamiltonian $T(p) = \frac{1}{2} p^T M^{-1} p$,

$$\dot{q} = M^{-1} p, \quad \dot{p} = 0. \quad (5.30)$$

This system can be solved exactly as well. The exact flow is

$$\phi_t^T(q, p) = \begin{pmatrix} q + t M^{-1} p \\ p \end{pmatrix}. \quad (5.31)$$

As ϕ_t^U and ϕ_t^T are exact flows of the respective Hamiltonian, they are both symplectic. We see that the compositions of ϕ_t^U and ϕ_t^T correspond to the symplectic Euler methods for separable Hamiltonians,

$$\varphi_h^A = \phi_h^U \circ \phi_h^T, \quad \varphi_h^B = \phi_h^T \circ \phi_h^U, \quad (5.32)$$

where φ_h^A and φ_h^B denote the numerical flows of symplectic Euler-A and symplectic Euler-B, respectively. As the Störmer-Verlet methods are compositions of the symplectic Euler methods, they are also splitting methods, corresponding to the compositions

$$\varphi_h^{SV1} = \varphi_{h/2}^A \circ \varphi_{h/2}^B = \phi_{h/2}^U \circ \phi_h^T \circ \phi_{h/2}^U, \quad (5.33a)$$

$$\varphi_h^{SV2} = \varphi_{h/2}^B \circ \varphi_{h/2}^A = \phi_{h/2}^T \circ \phi_h^U \circ \phi_{h/2}^T, \quad (5.33b)$$

respectively. This particular splitting is often referred to as *Strang splitting*.

Remark 5.4. *Let us note that not all symplectic integrators can be obtained as splitting methods. For the symplectic Euler methods and the Störmer-Verlet methods, this is only possible for separable Hamiltonian systems. For general Hamiltonians, these methods cannot be obtained from any splitting but are nevertheless symplectic.*

5.3.2 Fourth Order Methods

The general form of a fourth order symplectic integrator for separable Hamiltonian systems is given by

$$q_1 = q_0 + b_1 h T_p(p_0), \quad p_1 = p_0 - \hat{b}_1 h U_x(q_1), \quad (5.34a)$$

$$q_2 = q_1 + b_2 h T_p(p_1), \quad p_2 = p_1 - \hat{b}_2 h U_x(q_2), \quad (5.34b)$$

$$q_3 = q_2 + b_3 h T_p(p_2), \quad p_3 = p_2 - \hat{b}_3 h U_x(q_3), \quad (5.34c)$$

$$q_4 = q_3 + b_4 h T_p(p_3), \quad p_4 = p_3 - \hat{b}_4 h U_x(q_4). \quad (5.34d)$$

The quantities (q_0, p_0) are initial values and (q_4, p_4) are the numerical solution after one time step h . The whole algorithm can be written as

$$\varphi_h = \varphi_{\hat{b}_4 h}^U \circ \varphi_{b_4 h}^T \circ \varphi_{\hat{b}_3 h}^U \circ \varphi_{b_3 h}^T \circ \varphi_{\hat{b}_2 h}^U \circ \varphi_{b_2 h}^T \circ \varphi_{\hat{b}_1 h}^U \circ \varphi_{b_1 h}^T \quad (5.35)$$

and is therefore immediately seen to be symplectic. Two methods of fourth order are given by

$$b_1 = b_4 = \frac{1}{2(2-\gamma)}, \quad b_2 = b_3 = \frac{1-\gamma}{2(2-\gamma)}, \quad (5.36a)$$

$$\hat{b}_1 = \hat{b}_3 = \frac{1}{2-\gamma}, \quad \hat{b}_2 = -\frac{\gamma}{2-\gamma}, \quad \hat{b}_4 = 0, \quad (5.36b)$$

and

$$b_1 = 0, \quad b_2 = b_4 = \frac{1}{2-\gamma}, \quad b_3 = \frac{1}{1-\gamma^2}, \quad (5.37a)$$

$$\hat{b}_1 = \hat{b}_4 = \frac{1}{6}(2+\gamma+\gamma^{-1}), \quad \hat{b}_2 = \hat{b}_3 = \frac{1}{6}(2-\gamma-\gamma^{-1}), \quad (5.37b)$$

where $\gamma = 2^{1/3}$. Both methods are explicit and symmetric as either $\varphi_{\hat{b}_4 h}^U$ or $\varphi_{b_1 h}^T$ corresponds to the identity.

5.4 Higher Order Methods by Composition

The composition of a one-step symplectic integrator φ_h with different step sizes provides a simple way of obtaining higher order schemes. We assume that the initial scheme φ_h is symmetric, that is

$$\varphi_h \circ \varphi_{-h} = \text{id}, \quad (5.38)$$

as this simplifies the construction. A symmetric method can always be built by combining a non-symmetric method with its adjoint. If a numerical method φ_h is symmetric, it can be used to compose higher order methods by splitting up each timestep into s substeps [31, 58, 56],

$$\varphi_h = \varphi_{\gamma_s h} \circ \dots \circ \varphi_{\gamma_i h} \circ \dots \circ \varphi_{\gamma_1 h}, \quad (5.39)$$

where the careful selection of the γ_i is crucial for the performance of the resulting scheme. In the following, we present some fourth and sixth order composition methods that can be applied in most situations.

5.4.1 Fourth Order Composition Methods

If φ_h is a method of order r , a method $\hat{\varphi}_h$ of order $r + 2$ is obtained by the composition [31, Section V.3.2]

$$\hat{\varphi}_h = \varphi_{\gamma h} \circ \varphi_{(1-2\gamma)h} \circ \varphi_{\gamma h} \quad \text{with} \quad \gamma = (2 - 2^{1/(r+1)})^{-1}. \quad (5.40)$$

Hence, if φ_h is of second order, the resulting method $\hat{\varphi}_h$ will be of fourth order. Note that symmetric methods are always of even order. A method of the same order but with generally smaller errors is obtained by considering five steps

$$\hat{\varphi}_h = \varphi_{\gamma h} \circ \varphi_{\gamma h} \circ \varphi_{(1-4\gamma)h} \circ \varphi_{\gamma h} \circ \varphi_{\gamma h} \quad \text{with} \quad \gamma = (4 - 4^{1/(r+1)})^{-1}. \quad (5.41)$$

Multiple application of these compositions yields methods of orders higher than four.

5.4.2 Sixth Order Composition Methods

Higher order compositions can also be constructed directly [31, Section V.3.2]. A sixth order method with seven substeps is given by

$$\begin{aligned} \gamma_1 &= \gamma_7 = +0.78451361047755726381949763, \\ \gamma_2 &= \gamma_6 = +0.23557321335935813368479318, \\ \gamma_3 &= \gamma_5 = -1.17767998417887100694641568, \\ \gamma_4 &= +1.31518632068391121888424973, \end{aligned} \quad (5.42)$$

but again smaller errors can be achieved by using nine steps

$$\begin{aligned} \gamma_1 &= \gamma_9 = +0.39216144400731413927925056, \\ \gamma_2 &= \gamma_8 = +0.33259913678935943859974864, \\ \gamma_3 &= \gamma_7 = -0.70624617255763935980996482, \\ \gamma_4 &= \gamma_6 = +0.08221359629355080023149045, \\ \gamma_5 &= +0.79854399093482996339895035. \end{aligned} \quad (5.43)$$

The computational effort of these high order methods is quite large. Each step requires the solution of a nonlinear system of equations. Given the outstanding performance already second order symplectic integrators are able to deliver, the necessity for such high order methods is probably rarely found. Nevertheless, if extremely high accuracy is indispensable, these methods can be applied.

5.5 Symplectic Runge-Kutta Methods

Runge-Kutta methods with s internal stages $Z_{n,i}$ located at $t_n + c_i h$ have the form

$$\dot{Z}_{n,i} = \Omega^{-T} \nabla H(Z_{n,i}), \quad Z_{n,i} = z_n + h \sum_{j=1}^s a_{ij} \dot{Z}_{n,j}, \quad z_{n+1} = z_n + h \sum_{j=1}^s b_j \dot{Z}_{n,j}. \quad (5.44)$$

The constants c_i , b_i and a_{ij} , are the nodes, the weights, and the coefficients of the method, respectively. They determine the Runge-Kutta method and are usually summarised in the Butcher tableau,

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array} \quad (5.45)$$

A Runge-Kutta method is symplectic if the coefficients satisfy

$$b_i a_{ij} + b_j a_{ji} = b_i b_j. \quad (5.46)$$

Such methods are always implicit (at least diagonally) as for $i = j$ the symplecticity condition (5.46) becomes $2a_{ii} = b_i$ for $b_i \neq 0$, which implies that at least some diagonal entries of the Butcher tableau do not vanish.

Remark 5.5. *An diagonally implicit Runge-Kutta method φ_h satisfying the symplecticity condition (5.46) and $b_i \neq 0$ is equivalent to the composition*

$$\varphi_h = \varphi_{b_s h}^{\text{MP}} \circ \cdots \circ \varphi_{b_2 h}^{\text{MP}} \circ \varphi_{b_1 h}^{\text{MP}}, \quad (5.47)$$

where φ_h^{MP} stands for the implicit midpoint method.

An example for symplectic Runge-Kutta methods are Gauss-Legendre methods which are of order $p = 2s$, that is the optimal order obtainable for a given number of stages among all possible symplectic collocation Runge-Kutta methods. For the one-stage second-order method (implicit midpoint), the Butcher tableau is

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array} \quad (5.48)$$

For the two-stage fourth-order method, the Butcher tableau is

$$\begin{array}{c|cc} \frac{1}{2} - \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{4} - \frac{1}{6}\sqrt{3} \\ \frac{1}{2} + \frac{1}{6}\sqrt{3} & \frac{1}{4} + \frac{1}{6}\sqrt{3} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \quad (5.49)$$

As the Butcher tableaux are full, these are nonlinearly implicit methods and we have to solve them either by fixed-point iteration or by Newton's method.

5.5.1 Symplecticity

We discuss two proofs of symplecticity for Runge-Kutta methods. The first is based on the observation that symplecticity is equivalent to conservation of a quadratic invariant. Therefore all Runge-Kutta methods which preserve quadratic invariants are automatically symplectic. The second proof is based on linearisation of the integrator, similar to the proof for the symplectic Euler methods, Equations (5.17a)-(5.19).

Quadratic Invariants

This proof is taken from Hairer, Lubich, and Wanner [31, Sections VI.4 and IV.2] and follows Bochev and Scovel [8]. The proof of the symplecticity criterion (5.46) has two parts. First, we show that the numerical result (z_{n+1}, Ψ_{n+1}) , obtained from applying the method to the problem augmented by its variational equation, is equal to the numerical solution for $\dot{z} = f(z)$ augmented by its derivative $\dot{\Psi} = \partial z_{n+1} / \partial z_0$. Then we use the fact that symplecticity corresponds to conservation of a quadratic invariant, which is expressed in terms of the derivative $\Psi = dF_H^t / d\zeta(z_0)$, so that we can reduce the proof of symplecticity to proving conservation of quadratic invariants. The first step is summarised in the following lemma.

Lemma 5.6. *Runge-Kutta methods and partitioned Runge-Kutta methods are closed under differentiation, that is the following diagram commutes:*

$$\begin{array}{ccc}
 \dot{z} = f(z) = \Omega \nabla H(z), z(0) = z_0 & \xrightarrow{\text{method}} & z_{n+1} = \varphi_h(z_n) \\
 \downarrow \partial / \partial z_0 & & \downarrow \partial / \partial z_0 \\
 \dot{z} = f(z) = \Omega \nabla H(z), z(0) = z_0, \\
 \dot{\Psi} = f'(z)\Psi = \Omega \nabla^2 H(z)\Psi & \xrightarrow{\text{method}} & z_{n+1} = \varphi_h(z_n), \\
 & & \Psi_{n+1} = D\varphi_h(z_n)\Psi_n
 \end{array}$$

Proof. The proof follows by implicit differentiation. Let us illustrate this for the explicit Euler method

$$z_{n+1} = z_n + hf(z_n). \quad (5.50)$$

We consider z_n and z_{n+1} as functions of z_0 , and we differentiate with respect to z_0 the equation defining the numerical method. For the Euler method, this gives

$$\frac{\partial z_{n+1}}{\partial z_0} = \frac{\partial z_n}{\partial z_0} + hf'(z_n) \frac{\partial z_n}{\partial z_0}, \quad (5.51)$$

which rewritten in terms of Ψ ,

$$\Psi_{n+1} = \Psi_n + hf'(z_n)\Psi_n, \quad (5.52)$$

is exactly the relation that we get from applying the method to the variational equation. Since $\partial z_0 / \partial z_0 = \mathbb{1}$, we have $\partial z_n / \partial z_0 = \Psi_n$ for all n . \square

Observe that the symplecticity condition (5.2), written as

$$\Psi^T \Omega \Psi = \Omega, \quad (5.53)$$

is a quadratic first integral of the variational equations. Write the Hamiltonian system together with its variational equation as

$$\dot{z} = \Omega \nabla H(z), \quad \dot{\Psi} = \Omega \nabla^2 H(z) \Psi. \quad (5.54)$$

It follows from

$$\frac{d}{dt}(\Psi^T \Omega \Psi) = (\Omega \nabla^2 H(z) \Psi)^T \Omega \Psi + \Psi^T \Omega (\Omega \nabla^2 H(z) \Psi) = 0 \quad (5.55)$$

that $\Psi^T \Omega \Psi$ is a quadratic first integral of the augmented system (5.54). Therefore, every Runge-Kutta method that preserves quadratic first integrals, is a symplectic integrator. We set $y = (z, \Psi)$ and consider the quadratic invariant $Q(y) = y^T C y$ with

$$C = \begin{pmatrix} 0 & 0 \\ 0 & \Omega \end{pmatrix}. \quad (5.56)$$

With that the proof of the following theorem proves the symplecticity condition (5.46).

Theorem 5.7. *If the coefficients of a Runge-Kutta method satisfy*

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \quad \text{for all } i, j = 1, \dots, s, \quad (5.57)$$

then it conserves quadratic invariants $Q(y) = y^T C y$, where C is a (symmetric or skew-symmetric) square matrix and $y^T C f(y) + f(y)^T C y = 0$ for all y .

Proof. The relation $y_1 = y_0 + h \sum_{i=1}^s b_i F_i$ with $F_i = f(Y_i)$ and $Y_i = y_0 + h \sum_{j=1}^s a_{ij} F_j$ yields

$$y_1^T C y_1 = y_0^T C y_0 + h \sum_{i=1}^s b_i F_i^T C y_0 + h \sum_{j=1}^s b_j y_0^T C F_j + h^2 \sum_{i,j=1}^s b_i b_j F_i^T C F_j. \quad (5.58)$$

Compute y_0 from the relation for Y_i and insert into the central expressions of the previous equation,

$$\begin{aligned} y_1^T C y_1 &= y_0^T C y_0 + h \sum_{i=1}^s b_i F_i^T C \left(Y_i - h \sum_{j=1}^s a_{ij} F_j \right) \\ &\quad + h \sum_{j=1}^s b_j \left(Y_j - h \sum_{i=1}^s a_{ji} F_i \right)^T C F_j + h^2 \sum_{i,j=1}^s b_i b_j F_i^T C F_j \\ &= y_0^T C y_0 + h \sum_{i=1}^s b_i \left(F_i^T C Y_i + Y_i^T C F_i \right) + h^2 \sum_{i,j=1}^s \left(b_i b_j - b_i a_{ij} - b_j a_{ji} \right) F_i^T C F_j. \end{aligned} \quad (5.59)$$

Under the assumption that $y^T C y$ is an invariant so that $y^T C f(y) + f(y)^T C y = 0$ and that condition (5.57) is satisfied, we see that $y_1^T C y_1 = y_0^T C y_0$. \square

Linearisation

An alternative proof follows by linearisation of the integrator (see Leimkuhler and Reich [48, Section 6.3]). For this proof, we write (5.44) in terms of (q, p) ,

$$\dot{Q}_{n,i} = \frac{\partial H}{\partial p}(Q_{n,i}, P_{n,i}), \quad Q_{n,i} = q_n + h \sum_{j=1}^s a_{ij} \dot{Q}_{n,j}, \quad q_{n+1} = q_n + h \sum_{j=1}^s b_j \dot{Q}_{n,j}, \quad (5.60a)$$

$$\dot{P}_{n,i} = -\frac{\partial H}{\partial x}(Q_{n,i}, P_{n,i}), \quad P_{n,i} = p_n + h \sum_{j=1}^s a_{ij} \dot{P}_{n,j}, \quad p_{n+1} = p_n + h \sum_{j=1}^s b_j \dot{P}_{n,j}. \quad (5.60b)$$

Denote by $e = [1, 1, \dots, 1]^T$ the unit column vector with s rows and by $\mathbb{1}$ the $d \times d$ identity matrix. In order to write equations (5.60) in a more compact form, we associate with any s -stage Runge-Kutta method the $s \times s$ matrix $A = \{a_{ij}\}$ and the column vector $b = \{b_i\}$ with corresponding diagonal matrix B defined by $Be = b$. In the following, we make use of the tensor product notation (see Van Loan [74]). The tensor product $T \otimes S$ of an arbitrary $m \times m$ matrix $T = \{t_{ij}\}$ and an arbitrary $n \times n$ matrix $S = \{s_{ij}\}$ is a $k \times k$ matrix, $k = mn$, defined by

$$T \otimes S = \begin{pmatrix} t_{11}S & t_{12}S & \dots & t_{1m}S \\ t_{21}S & t_{22}S & \dots & t_{2m}S \\ \vdots & & \ddots & \vdots \\ t_{m1}S & t_{m2}S & \dots & t_{mm}S \end{pmatrix}. \quad (5.61)$$

Two important properties of such tensor products are

$$(R \otimes S)(T \otimes U) = (RT) \otimes (SU), \quad (R \otimes S)^T = (R^T \otimes S^T), \quad (5.62)$$

whenever the products are defined. In this notation, the Runge-Kutta method (5.60) can be rewritten as

$$Q = e \otimes q_n + h(A \otimes \mathbb{1})F, \quad q_{n+1} = q_n + h(b^T \otimes \mathbb{1})F, \quad (5.63a)$$

$$P = e \otimes p_n + h(A \otimes \mathbb{1})G, \quad p_{n+1} = p_n + h(b^T \otimes \mathbb{1})G, \quad (5.63b)$$

where $Q, P, F, G \in \mathbb{R}^{sd}$ are given by

$$Q = \begin{pmatrix} Q_{n,1} \\ Q_{n,2} \\ \vdots \\ Q_{n,s} \end{pmatrix}, \quad P = \begin{pmatrix} P_{n,1} \\ P_{n,2} \\ \vdots \\ P_{n,s} \end{pmatrix}, \quad F = \begin{pmatrix} H_p(Q_{n,1}, P_{n,1}) \\ H_p(Q_{n,2}, P_{n,2}) \\ \vdots \\ H_p(Q_{n,s}, P_{n,s}) \end{pmatrix}, \quad G = \begin{pmatrix} -H_x(Q_{n,1}, P_{n,1}) \\ -H_x(Q_{n,2}, P_{n,2}) \\ \vdots \\ -H_x(Q_{n,s}, P_{n,s}) \end{pmatrix}. \quad (5.64)$$

With that, the linearisation of the Runge-Kutta method (5.60) is implicitly given by the system

$$dQ = e \otimes dq_n + h(A \otimes \mathbb{1})dF, \quad dq_{n+1} = dq_n + h(b^T \otimes \mathbb{1})dF, \quad (5.65a)$$

$$dP = e \otimes dp_n + h(A \otimes \mathbb{1})dG, \quad dp_{n+1} = dp_n + h(b^T \otimes \mathbb{1})dG, \quad (5.65b)$$

where

$$dF = F_x dQ + F_p dP, \quad dG = G_x dQ + G_p dP. \quad (5.66)$$

As we are considering a Hamiltonian system, we have

$$F_x^T = -G_p, \quad F_p = F_p^T, \quad G_x = G_x^T. \quad (5.67)$$

Compute the wedge product of dq_{n+1} and dp_{n+1} ,

$$\begin{aligned} dq_{n+1} \wedge dp_{n+1} &= dq_n \wedge dp_n - h dp_n \wedge (b^T \otimes \mathbb{1})dF + h dq_n \wedge (b^T \otimes \mathbb{1})dG \\ &\quad + h^2 (b^T \otimes \mathbb{1})dF \wedge (b^T \otimes \mathbb{1})dG. \end{aligned} \quad (5.68)$$

Using

$$(b^T \otimes \mathbb{1})dF \wedge (b^T \otimes \mathbb{1})dG = dF \wedge (b^T \otimes \mathbb{1})^T (b^T \otimes \mathbb{1})dG = dF \wedge (bb^T \otimes \mathbb{1})dG, \quad (5.69)$$

we obtain

$$\begin{aligned} dq_{n+1} \wedge dp_{n+1} &= dq_n \wedge dp_n - h dp_n \wedge (b^T \otimes \mathbb{1}) dF + h dq_n \wedge (b^T \otimes \mathbb{1}) dG \\ &\quad + h^2 dF \wedge (bb^T \otimes \mathbb{1}) dG. \end{aligned} \quad (5.70)$$

From dQ and dP in (5.65), we obtain

$$\begin{aligned} dQ \wedge (B \otimes \mathbb{1}) dG &= e \otimes dq_n \wedge (B \otimes \mathbb{1}) dG + h (A \otimes \mathbb{1}) dF \wedge (B \otimes \mathbb{1}) dG \\ &= dq_n \wedge (b^T \otimes \mathbb{1}) dG + h dF \wedge (A^T B \otimes \mathbb{1}) dG, \end{aligned} \quad (5.71a)$$

$$\begin{aligned} dP \wedge (B \otimes \mathbb{1}) dF &= e \otimes dp_n \wedge (B \otimes \mathbb{1}) dF + h (A \otimes \mathbb{1}) dG \wedge (B \otimes \mathbb{1}) dF \\ &= dp_n \wedge (b^T \otimes \mathbb{1}) dF - h dF \wedge (B^T A \otimes \mathbb{1}) dG. \end{aligned} \quad (5.71b)$$

Equations (5.71) can be used to replace the second and third term on the right-hand side of Equation (5.70),

$$\begin{aligned} dq_{n+1} \wedge dp_{n+1} &= dq_n \wedge dp_n - h dP \wedge (B \otimes \mathbb{1}) dF + h dQ \wedge (B \otimes \mathbb{1}) dG \\ &\quad + h^2 dF \wedge ([bb^T - B^T A - A^T B] \otimes \mathbb{1}) dG. \end{aligned} \quad (5.72)$$

Because of (5.67), we have

$$\begin{aligned} dQ \wedge (B \otimes \mathbb{1}) dG - dP \wedge (B \otimes \mathbb{1}) dF &= dQ \wedge (B \otimes \mathbb{1}) G_p dP - dP \wedge (B \otimes \mathbb{1}) F_x dQ \\ &= dQ \wedge (B \otimes \mathbb{1}) (G_p + F_x^T) dP = 0, \end{aligned} \quad (5.73)$$

so that

$$dq_{n+1} \wedge dp_{n+1} = dq_n \wedge dp_n + h^2 dF \wedge ([bb^T - B^T A - A^T B] \otimes \mathbb{1}) dG. \quad (5.74)$$

We therefore have

$$dq_{n+1} \wedge dp_{n+1} = dq_n \wedge dp_n, \quad (5.75)$$

if

$$bb^T - B^T A - A^T B = 0, \quad (5.76)$$

which is equivalent to the symplecticity condition (5.46).

5.6 Symplectic-Partitioned Runge-Kutta Methods

Partitioned Runge-Kutta methods with s internal stages (Q_i, P_i) located at $t_n + c_i h$ have the form

$$\dot{Q}_{n,i} = \frac{\partial H}{\partial p}(Q_{n,i}, P_{n,i}), \quad Q_{n,i} = q_n + h \sum_{j=1}^s a_{ij} \dot{Q}_{n,j}, \quad q_{n+1} = q_n + h \sum_{j=1}^s b_j \dot{Q}_{n,j}, \quad (5.77a)$$

$$\dot{P}_{n,i} = -\frac{\partial H}{\partial x}(Q_{n,i}, P_{n,i}), \quad P_{n,i} = p_n + h \sum_{j=1}^s \bar{a}_{ij} \dot{P}_{n,j}, \quad p_{n+1} = p_n + h \sum_{j=1}^s \bar{b}_j \dot{P}_{n,j}. \quad (5.77b)$$

The method is symplectic if the coefficients satisfy

$$b_i \bar{a}_{ij} + \bar{b}_j a_{ji} = b_i \bar{b}_j \quad \text{and} \quad b_i = \bar{b}_i. \quad (5.78)$$

Interestingly, partitioned Runge-Kutta methods can be explicit and symmetric for separable Hamiltonian systems. However, for separable Hamiltonians, symplectic-partitioned Runge-Kutta methods can always be obtained by splitting or composition. In fact, the methods of (5.36) and (5.37) are symplectic-partitioned Runge-Kutta methods with Butcher tableaux

$$\begin{array}{c|cccc} b_1 & 0 & 0 & 0 & \\ b_1 & b_2 & 0 & 0 & \\ b_1 & b_2 & b_3 & 0 & \\ \hline b_1 & b_2 & b_3 & b_4 & \end{array} \quad \text{and} \quad \begin{array}{c|cccc} \hat{b}_1 & 0 & 0 & 0 & \\ \hat{b}_1 & \hat{b}_2 & 0 & 0 & \\ \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & 0 & \\ \hline \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \hat{b}_4 & \\ \hline \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \hat{b}_4 & \end{array} . \quad (5.79)$$

Other symplectic-partitioned Runge-Kutta methods are the Lobatto-IIIA-IIIB pairs, which interestingly are not symplectic on their own, when considered individually, just like the explicit and implicit Euler methods. The second-order Lobatto-IIIA-IIIB method, with Butcher tableaux

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \quad \text{and} \quad \begin{array}{c|cc} 0 & \frac{1}{2} & 0 \\ 1 & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \quad (5.80)$$

is just the leapfrog scheme. Another second-order scheme is provided by the Lobatto-IIIC method with Butcher tableau

$$\begin{array}{c|cc} 0 & \frac{1}{2} & -\frac{1}{2} \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \quad (5.81)$$

for both a_{ij} and \bar{a}_{ij} . The proof of symplecticity is omitted here as it follows in a similar way as for non-partitioned Runge-Kutta methods. Later on, we will see that the partitioned-symplectic Runge-Kutta methods can be obtained from a discrete variational principle which immediately implies their symplecticity.

Remark 5.8. *Symplectic-partitioned Runge-Kutta methods exactly preserve first integrals of the form*

$$I = q^T W p + d_1^T q + d_2^T p, \quad (5.82)$$

where W is a constant $d \times d$ matrix and $d_1, d_2 \in \mathbb{R}^d$ are two vectors.

First integrals of this type arise from the symmetry of the Hamiltonian H under a linear canonical point transformation. For systems with pairwise distance-dependent interactions (e.g., N-body systems), these integrals include the total linear and angular momentum.

6 Volume Preserving Integrators

Volume preserving methods are useful for integrating Hamiltonian systems, where phasespace volume is preserved, but also for more general equations with divergence free vector fields. Recall that the vector field f of the d dimensional ODE

$$\dot{z} = f(z) \quad (6.1)$$

is divergence-free if

$$\nabla \cdot f = \sum_{i=1}^d \frac{\partial f_i}{\partial z^i} = \text{tr}(f') = 0 \quad \text{for all } z, \quad (6.2)$$

where f' denotes the Jacobian of f . Let Φ_t be the exact flow of (6.1) and $J = \Phi'_t$ its Jacobian. The volume of some domain $\Omega \in \mathbb{R}^d$ is given by

$$\text{vol } \Omega = \int_{\Omega} dz. \quad (6.3)$$

Under the flow Φ_t the volume of Ω changes according to

$$\text{vol } \Phi_t(\Omega) = \int_{\Omega} |\det J| dz. \quad (6.4)$$

This implies that the map Φ_t preserves volume if $|\det J| = 1$.

Theorem 6.1 (Liouville's Theorem). *If the vector field f is divergence-free, its flow Φ_t is a volume-preserving map (for all t).*

Proof. We want to show that the volume of Ω is preserved under the flow of Φ_t if f is divergence-free. The flow map satisfies

$$\frac{d}{dt} \Phi_t(z) = f(\Phi_t(z)). \quad (6.5)$$

Differentiate the whole equation w.r.t. z to obtain

$$\frac{d}{dt} \Phi'_t(z) = f'(\Phi_t(z)) \Phi'_t(z), \quad (6.6)$$

that is J evolves according to

$$\dot{J} = f'(\Phi_t(z)) J. \quad (6.7)$$

Assuming that J is invertible, we can multiply this equation from the right by J^{-1} . Computing the trace of the result, we get

$$\text{tr}(\dot{J} J^{-1}) = \text{tr}(f'(\Phi_t(z))), \quad (6.8)$$

which vanishes if f is divergence-free. According to Jacobi's formula for the derivative of a determinant (*Abel–Liouville–Jacobi–Ostrogradskii identity*), we have

$$\frac{d}{dt}(\det J) = (\det J) \operatorname{tr}(\dot{J}J^{-1}), \quad (6.9)$$

which again vanishes if f is divergence-free. Since $\Phi_0 = \operatorname{id}$ so that $J(0) = \Phi'_0(z) = \mathbb{1}$, it follows that

$$\det J = \det \Phi'_t(z) = 1 \quad \text{for all } t \text{ and all } z, \quad (6.10)$$

which completes the proof. \square

6.1 Splitting Methods

A general algorithm for constructing volume-preserving methods is based on the following theorem.

Theorem 6.2. *Every divergence-free vector field $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ can be written as the sum of $d - 1$ vector fields*

$$f = f_{1,2} + f_{2,3} + \cdots + f_{d-1,d}, \quad (6.11)$$

where each $f_{i,i+1}$ is Hamiltonian in the variables (z^i, z^{i+1}) , that is there exist functions $H_{i,i+1} : \mathbb{R}^d \rightarrow \mathbb{R}$ such that

$$f_{i,i+1} = \left(0, \dots, 0, -\frac{\partial H_{i,i+1}}{\partial z^{i+1}}, \frac{\partial H_{i,i+1}}{\partial z^i}, 0, \dots, 0 \right)^T. \quad (6.12)$$

Proof. In terms of the components of $f = (f^1, f^2, \dots, f^d)^T$, the functions $H_{i,i+1}$ must satisfy the equations

$$f^1 = -\frac{\partial H_{1,2}}{\partial z^2}, \quad (6.13a)$$

$$f^2 = \frac{\partial H_{1,2}}{\partial z^1} - \frac{\partial H_{2,3}}{\partial z^3}, \quad (6.13b)$$

$$\vdots$$

$$f^{d-1} = \frac{\partial H_{d-2,d-1}}{\partial z^{d-2}} - \frac{\partial H_{d-1,d}}{\partial z^d}, \quad (6.13c)$$

$$f^d = \frac{\partial H_{d-1,d}}{\partial z^{d-1}}. \quad (6.13d)$$

In order to see this, write the first few vector fields $f_{1,2}$, etc.,

$$f_{1,2} = \left(-\frac{\partial H_{1,2}}{\partial z^2}, 0, 0, 0, 0, \dots, 0 \right)^T, \quad (6.14a)$$

$$f_{2,3} = \left(0, -\frac{\partial H_{2,3}}{\partial z^3}, \frac{\partial H_{2,3}}{\partial z^2}, 0, 0, \dots, 0 \right)^T, \quad (6.14b)$$

$$f_{3,4} = \left(0, 0, -\frac{\partial H_{3,4}}{\partial z^4}, \frac{\partial H_{3,4}}{\partial z^3}, 0, \dots, 0 \right)^T, \quad (6.14c)$$

$$\dots$$

We thus set

$$H_{1,2} = - \int_0^{z^2} f^1 dz^2, \quad (6.15a)$$

$$H_{i,i+1} = \int_0^{z^{i+1}} \left(\frac{\partial H_{i-1,i}}{\partial z^{i-1}} - f^i \right) dz^{i+1} \quad (2 \leq i \leq d-2). \quad (6.15b)$$

It remains to construct the last Hamiltonian $H_{d-1,d}$. By induction we see that for $i \leq d-2$,

$$\frac{\partial^2 H_{i,i+1}}{\partial z^i \partial z^{i+1}} = - \left(\frac{\partial f^1}{\partial z^1} + \cdots + \frac{\partial f^i}{\partial z^i} \right), \quad (6.16)$$

hence the integrability condition for $H_{d-1,d}$,

$$\frac{\partial}{\partial z^{d-1}} \left(\frac{\partial H_{d-2,d-1}}{\partial z^{d-2}} - f^{d-1} \right) = \frac{\partial f^d}{\partial z^d}, \quad (6.17)$$

reduces to the condition $\operatorname{div} f = 0$, which is satisfied by assumption. $H_{d-1,d}$ can thus be constructed as

$$H_{d-1,d} = \int_0^{z^d} \left(\frac{\partial H_{d-2,d-1}}{\partial z^{d-2}} - f^{d-1} \right) dz^d + \int_0^{z^{d-1}} f^d|_{z^d=0} dz^{d-1}, \quad (6.18)$$

which completes the proof. \square

The above construction also shows that

$$f_{i,i+1} = (0, \dots, 0, f^i + g^i, -g^{i+1}, 0, \dots, 0)^T, \quad (6.19)$$

with

$$g^1 = 0, \quad (6.20a)$$

$$g^{i+1} = \int_0^{z^{i+1}} \left(\frac{\partial f^1}{\partial z^1} + \cdots + \frac{\partial f^i}{\partial z^i} \right) \quad \text{for } 1 \leq i \leq d-2, \quad (6.20b)$$

$$g^d = -f^d. \quad (6.20c)$$

With the above decomposition, a volume-preserving algorithm is obtained by applying a splitting method with symplectic substeps, e.g., a second-order scheme is obtained by Strang splitting with symplectic Euler substeps,

$$\varphi_h = \varphi_{h/2}^{[1,2]*} \circ \cdots \circ \varphi_{h/2}^{[d-1,d]*} \circ \varphi_{h/2}^{[d-1,d]} \circ \cdots \circ \varphi_{h/2}^{[1,2]}, \quad (6.21)$$

where $\varphi_{h/2}^{[i,i+1]}$ is a symplectic Euler step of length $h/2$ applied to the system with right-hand side $f_{i,i+1}$ and $*$ denotes the adjoint method. Even though the methods $\varphi_{h/2}^{[i,i+1]}$ are not symplectic in the whole space \mathbb{R}^d , they are volume-preserving. In general, the method is one-dimensionally implicit, but becomes explicit in the particular case where $\partial f^i / \partial z^i = 0$ for all i .

6.2 Runge-Kutta Methods

An interesting result [38] from backward error analysis states that in order to integrate divergence-free vector fields whilst preserving volume, the modified equation of a Runge-Kutta method must be exactly the same as the original differential equation,

$$\dot{z} = \tilde{f}(z) = f(z). \quad (6.22)$$

This requirement is impossible to satisfy in general, which leads to the following theorem.

Theorem 6.3. *Runge-Kutta methods cannot preserve volume for a general divergence-free vector field.*

Proof. See Iserles, Quispel, and Tse [38]. □

Nevertheless, there are divergence-free vector fields with special structure for which particular Runge-Kutta methods are volume-preserving. Hairer, Lubich, and Wanner [31] show that Runge-Kutta methods with at most two stages are volume-preserving for divergence-free vector fields of the form $f(x, y) = (u(y), v(x))^T$ with $u : \mathbb{R}^n \rightarrow \mathbb{R}^m$ and $v : \mathbb{R}^m \rightarrow \mathbb{R}^n$ so that

$$\dot{x} = u(y), \quad \dot{y} = v(x). \quad (6.23)$$

For such a system, the splitting scheme of the previous section becomes the composition of the symplectic Euler method and its adjoint, that is the second-order Lobatto IIIA-IIIB pair. All explicit symplectic-partitioned Runge-Kutta methods are compositions of symplectic Euler steps ([31, Theorem VI.4.7]). Therefore this observation proves that such methods are volume-preserving for systems of the form (6.23). A more general statement is given by the following theorem.

Theorem 6.4. *Every symplectic Runge-Kutta method with at most two stages is volume-preserving for systems (6.23) of arbitrary dimension.*

Proof. See Hairer, Lubich, and Wanner [31, Section VI.9, Theorem 9.4]. □

Recently, more general conditions for Runge-Kutta methods to preserve volume for divergence-free vector fields satisfying

$$\det\left(\mathbb{1} + \frac{h}{2}f'(z)\right) = \det\left(\mathbb{1} - \frac{h}{2}f'(z)\right) \quad \text{for all } h > 0 \text{ and all } x \in \mathbb{R}^d, \quad (6.24)$$

which includes Hamiltonian systems as well as systems of the form (6.23), have been derived by Bader et al. [5].

7 Variational Integrators

The basic idea of variational integrators is to construct a discrete counterpart to a particular mechanical system instead of directly discretising its equations of motion. This means that the fundamental building blocks of classical mechanics, namely the action functional, the Lagrangian, the variational principle, and the Noether theorem, all have discrete equivalents. The application of the discrete variational principle to the discrete action then leads to discrete Euler-Lagrange equations. The evolution map that corresponds to the discrete Euler-Lagrange equations is what is called a variational integrator. The discrete Noether theorem can be used to relate symmetries of the discretised system to discrete momenta that are in principle exactly preserved by this integrator.

With standard numerical methods, one approximately solves the exact equations of some system. In a sense, here the idea is to exactly solve the equations of some approximate system.

The seminal work in the development of a discrete equivalent of classical mechanics was presented by Veselov [75, 76]. His method, based on a discrete variational principle, leads to symplectic integration schemes that automatically preserve constants of motion [77, 55]. A comprehensive review of discrete mechanics can be found in Marsden and West [56], including a thorough account on the historical development. The discrete version of Hamilton's phasespace action principle is presented in Leok and Zhang [50].

7.1 Discretisation of the Action

The derivation of the discrete theory follows along the lines of the derivation of the continuous theory. The starting point is the discretisation of the space of paths $\mathcal{Q}(\mathcal{M})$ that connect two points in \mathcal{M} ,

$$\mathcal{Q}(\mathcal{M}) = \{q : \mathcal{I} \rightarrow \mathcal{M} \mid \mathcal{I} \subset \mathbb{R} \text{ smooth and bounded}\}. \quad (7.1)$$

Therefore we divide each time interval \mathcal{I} into an equidistant, monotonic sequence $\{t_n\}_{n=0}^N$ and defined the discrete path space as

$$\mathcal{Q}_d(\mathcal{M}) = \{q_d : \{t_n\}_{n=0}^N \rightarrow \mathcal{M}\}. \quad (7.2)$$

The space $\mathcal{Q}_d(\mathcal{M})$ contains all possible discrete trajectories q_d in \mathcal{M} and is isomorphic to $\mathcal{M} \times \dots \times \mathcal{M}$ ($N+1$ copies),

$$\mathcal{Q}_d(\mathcal{M}) \cong \bigtimes_{N+1} \mathcal{M}. \quad (7.3)$$

Therefore $\mathcal{Q}_d(\mathcal{M})$ constitutes a finite-dimensional approximation of the infinite-dimensional space $\mathcal{Q}(\mathcal{M})$. Fixing an interval $[0, T]$, so that

$$\{t_n\}_{n=0}^N = \{t_n = nh \mid n = 0, \dots, N, Nh = T\} \subset \mathbb{R}, \quad (7.4)$$

is an increasing sequence of time points and h is the discrete time step, the discrete equivalent of the space of curves from q_0 to q_N ,

$$\mathcal{Q}(q_0, q_N, [0, T]) = \{q : [0, T] \rightarrow \mathcal{M} \mid q(0) = q_0, q(T) = q_N\} \subset \mathcal{Q}(\mathcal{M}), \quad (7.5)$$

is the space that contains all discrete trajectories with fixed endpoints q_0 and q_N , defined as

$$\mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N) = \{q_d : \{t_n\}_{n=0}^N \rightarrow \mathcal{M} \mid q(t_0) = q_0, q(t_N) = q_N\} \subset \mathcal{Q}_d(\mathcal{M}). \quad (7.6)$$

The discrete trajectory can be written as $q_d = \{q_n\}_{n=0}^N$, where q_n denotes the generalised coordinates at time t_n . The space $\mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N)$ is a finite-dimensional approximation of $\mathcal{Q}(q_0, q_N, [0, T])$. In the following, we will use piecewise linear Lagrange polynomials to approximate the trajectory $q(t)$, that is

$$q_h(t)|_{[t_n, t_{n+1}]} = q_n \frac{t_{n+1} - t}{t_{n+1} - t_n} + q_{n+1} \frac{t - t_n}{t_{n+1} - t_n}. \quad (7.7)$$

The next step is to choose a quadrature rule which determines the discrete action. While the continuous action is a map

$$\mathcal{A} : \mathcal{Q}(q_0, q_N, [0, T]) \rightarrow \mathbb{R}, \quad (7.8)$$

assigning real values to each path $q(t)$, the discrete action is a map

$$\mathcal{A}_d : \mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N) \rightarrow \mathbb{R}, \quad (7.9)$$

assigning real values to each discrete path q_d . Once we obtained the discrete action, everything else follows in a straight forward and systematic way from Hamilton's principle of stationary action, so that these choices are determining the form of the discrete equations of motion.

After we fix the sequence $\{t_n\}_{n=0}^N$, the continuous action can be written as

$$\mathcal{A}[q(t)] = \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} L(q, \dot{q}) dt. \quad (7.10)$$

The terms of the sum are called the *exact discrete Lagrangian*,

$$L_d^e(q_n, q_{n+1}) = \int_{t_n}^{t_{n+1}} L(q_{n,n+1}(t), \dot{q}_{n,n+1}(t)) dt, \quad (7.11)$$

which is defined as a function of two consecutive points on the discrete trajectory $q_d = \{q_n\}_{n=0}^N$. Here, $q_{n,n+1}(t)$ denotes the solution of the continuous Euler-Lagrange equations in the interval $[t_n, t_{n+1}]$ satisfying the boundary conditions $q_{n,n+1}(t_n) = q_n$ and $q_{n,n+1}(t_{n+1}) = q_{n+1}$, with q_n denoting the generalised coordinates at time t_n and \dot{q}_n the generalised velocities at time point t_n . In practice, the exact discrete Lagrangian cannot be computed exactly, which means we have to approximate it,

$$L_d(q_n, q_{n+1}) \approx \int_{t_n}^{t_{n+1}} L(q_{n,n+1}(t), \dot{q}_{n,n+1}(t)) dt. \quad (7.12)$$

That is, we have to approximate the trajectory $q(t)$, the velocity $\dot{q}(t)$ and the integral. This approximation leads to the discrete Lagrangian, given as

$$L_d(q_n, q_{n+1}) = h \sum_{i=1}^s b_i L(q_h(t_n + c_i h), \dot{q}_h(t_n + c_i h)), \quad (7.13)$$

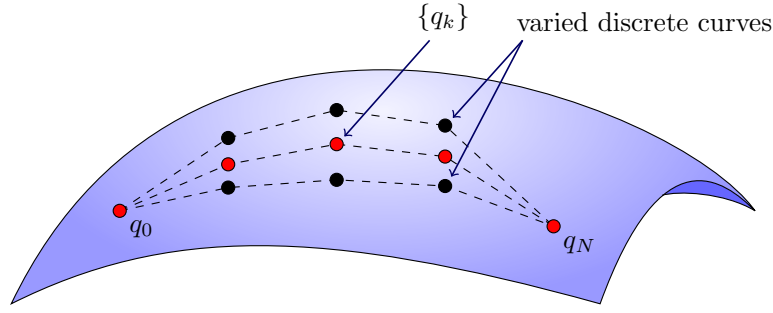


Fig. 7.1: Variations of the discrete trajectory $\{q_n\}_{n=0}^N$.

where $q_n = q_h(t_n)$ and $q_{n+1} = q_h(t_{n+1})$. The discrete action thus becomes merely a sum over the time index of discrete Lagrangians

$$\mathcal{A}_d[q_d] = \sum_{n=0}^{N-1} L_d(q_n, q_{n+1}), \quad (7.14)$$

which defines a map $\mathcal{A}_d : \mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N) \rightarrow \mathbb{R}$. In order to obtain the discrete Lagrangian, the generalised velocities are often discretised by simple finite-difference expressions¹, i.e.,

$$\dot{q}(t) \approx \frac{q_{n+1} - q_n}{h} \quad \text{for} \quad t \in [t_n, t_{n+1}]. \quad (7.15)$$

This corresponds to approximating the trajectory $q(t)$ between t_n and t_{n+1} by linear interpolation between q_n and q_{n+1} like in (7.7) and taking the derivative of $q_h(t)$ with respect to t . The quadrature is most often realised by either the trapezoidal rule ($c_1 = 0$, $c_2 = 1$),

$$L_d^{\text{tr}}(q_n, q_{n+1}) = \frac{h}{2} L\left(q_n, \frac{q_{n+1} - q_n}{h}\right) + \frac{h}{2} L\left(q_{n+1}, \frac{q_{n+1} - q_n}{h}\right), \quad (7.16)$$

or the midpoint rule ($c_1 = 1/2$),

$$L_d^{\text{mp}}(q_n, q_{n+1}) = h L\left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{h}\right). \quad (7.17)$$

The configuration manifold of the discrete theory is still \mathcal{M} , but the discrete state space is $\mathcal{M} \times \mathcal{M}$ instead of $\text{T}\mathcal{M}$, such that the discrete Lagrangian L_d is a function

$$L_d : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R}, \quad (7.18)$$

mapping two points on the discrete trajectory into the real numbers.

7.2 Discrete Euler-Lagrange Equations

The discrete trajectories $q_d = \{q_n\}_{n=0}^N$ are required to satisfy a discrete version of Hamilton's principle of stationary action

$$\delta \mathcal{A}_d[q_d] = \delta \sum_{n=0}^{N-1} L_d(q_n, q_{n+1}) = 0. \quad (7.19)$$

¹In the first term of the trapezoidal rule (7.16), this corresponds to a forward finite-difference, in the second term to a backward finite-difference, and in the midpoint rule (7.17) to a centred finite-difference.

As each point q_n of the discrete trajectory takes continuous values, we consider variations as one-parameter families of transformations, that is families of paths $q_d^\epsilon = \{q_n^\epsilon\}_{n=0}^N \in \mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N)$ which contain the solution path q_d for $\epsilon = 0$. The variations of q_d are contained in the tangent space $\mathbb{T}_{q_d} \mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N)$ to $\mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N)$ at q_d . It is defined as the set of maps

$$v_{q_d} : \{t_n\}_{n=0}^N \rightarrow \mathbb{T}\mathcal{M} \quad \text{such that} \quad \pi_{\mathcal{M}} \circ v_{q_d} = q_d \quad \text{and} \quad v(t_0) = v(t_N) = 0, \quad (7.20)$$

where $\pi_{\mathcal{M}}$ is the canonical projection $\pi_{\mathcal{M}} : \mathbb{T}\mathcal{M} \rightarrow \mathcal{M}$ and local coordinates are given by

$$v_{q_d} = \{(q_n, v_n)\}_{n=0}^N. \quad (7.21)$$

In particular, a discrete variation v_{q_d} of the discrete path q_d is defined as

$$v_{q_d} = \left. \frac{d}{d\epsilon} q_d^\epsilon \right|_{\epsilon=0}. \quad (7.22)$$

By identifying $\delta \equiv d/d\epsilon|_{\epsilon=0}$, we can also denote the variation by $v_{q_d} = \delta q_d$. In analogy to (4.30), the variation of the discrete action can be written as

$$\delta \mathcal{A}_d[q_d] = \left. \frac{d}{d\epsilon} \mathcal{A}_d[q_d^\epsilon] \right|_{\epsilon=0} = d\mathcal{A}_d[q_d] \cdot v_{q_d}, \quad (7.23)$$

which explicitly computed becomes

$$d\mathcal{A}_d[q_d] \cdot v_{q_d} = \sum_{n=0}^{N-1} [D_1 L_d(q_n, q_{n+1}) \cdot v_n + D_2 L_d(q_n, q_{n+1}) \cdot v_{n+1}], \quad (7.24)$$

where D_i denotes the derivative with respect to the i th argument (slot derivative). What follows corresponds to a discrete integration by parts, i.e., a reordering of the summation. The $n = 0$ term is separated from the first part of the sum and the $n = N - 1$ term is separated from the second part

$$\begin{aligned} d\mathcal{A}_d[q_d] \cdot v_{q_d} &= D_1 L_d(q_0, q_1) \cdot v_0 + \sum_{n=1}^{N-1} D_1 L_d(q_n, q_{n+1}) \cdot v_n \\ &\quad + \sum_{n=0}^{N-2} D_2 L_d(q_n, q_{n+1}) \cdot v_{n+1} + D_2 L_d(q_{N-1}, q_N) \cdot v_N. \end{aligned} \quad (7.25)$$

As the variations at the endpoints are kept fixed, $v_0 = v(t_0) = 0$ as well as $v_N = v(t_N) = 0$, the corresponding terms vanish. At last, the summation range of the second sum is shifted upwards by one with the arguments of the discrete Lagrangian adapted correspondingly

$$d\mathcal{A}_d[q_d] \cdot v_{q_d} = \sum_{n=1}^{N-1} [D_1 L_d(q_n, q_{n+1}) + D_2 L_d(q_{n-1}, q_n)] \cdot v_n. \quad (7.26)$$

Hamilton's principle of least action requires the variation of the discrete action $\delta \mathcal{A}_d$ to vanish for any choice of v_n . Consequently, the expression in the square brackets has to vanish. This defines the discrete Euler-Lagrange equations

$$D_1 L_d(q_n, q_{n+1}) + D_2 L_d(q_{n-1}, q_n) = 0 \quad (7.27)$$

The discrete Euler-Lagrange equations define an evolution map

$$\varphi_h : \mathcal{M} \times \mathcal{M} \rightarrow \mathcal{M} \times \mathcal{M} : (q_{n-1}, q_n) \mapsto (q_n, q_{n+1}). \quad (7.28)$$

Starting from two configurations, $q_0 \approx q(t_0)$ and $q_1 \approx q(t_1 = t_0 + h)$, the successive solution of the discrete Euler-Lagrange equations for q_2, q_3 , etc., up to q_N , determines the discrete trajectory $\{q_n\}_{n=0}^N$.

7.3 Discrete Fibre Derivative

Quite often it is more practical to prescribe an initial position and momentum instead of the configuration of the first two time steps. We therefore want to define the discrete momentum p_n at time step n . In the continuous setting this was done with the help of the fibre derivative. However, in the discrete setting, we have two ways to define discrete fibre derivatives,

$$\mathbb{F}^-L_d, \mathbb{F}^+L_d : \mathcal{M} \times \mathcal{M} \rightarrow T^*\mathcal{M}, \quad (7.29)$$

which map the discrete state space $\mathcal{M} \times \mathcal{M}$ to the tangent bundle $T^*\mathcal{M}$. They are given by

$$\mathbb{F}^-L_d : (q_n, q_{n+1}) \mapsto (q_n, p_n) = (q_n, -D_1L_d(q_n, q_{n+1})), \quad (7.30a)$$

$$\mathbb{F}^+L_d : (q_n, q_{n+1}) \mapsto (q_{n+1}, p_{n+1}) = (q_{n+1}, D_2L_d(q_n, q_{n+1})). \quad (7.30b)$$

The discrete Euler-Lagrange equations can now be rewritten as

$$\mathbb{F}^+L_d(q_{n-1}, q_n) = \mathbb{F}^-L_d(q_n, q_{n+1}), \quad (7.31)$$

that is

$$p_n = D_2L_d(q_{n-1}, q_n) = -D_1L_d(q_n, q_{n+1}). \quad (7.32)$$

Thus the discrete fibre derivatives permit a new interpretation of the discrete Euler–Lagrange equations. The variational integrator can be rewritten in position-momentum form,

$$p_n = -D_1L_d(q_n, q_{n+1}), \quad (7.33a)$$

$$p_{n+1} = D_2L_d(q_n, q_{n+1}). \quad (7.33b)$$

Given (q_n, p_n) , the first equation can be solved for q_{n+1} . This is generally a nonlinearly implicit equation that has to be solved by some iterative technique like Newton's method. The second equation is an explicit function, so to obtain p_{n+1} we merely have to plug in q_n and q_{n+1} . The corresponding Hamiltonian evolution map is

$$\tilde{\varphi}_h : T^*\mathcal{M} \rightarrow T^*\mathcal{M} : (q_n, p_n) \mapsto (q_{n+1}, p_{n+1}). \quad (7.34)$$

Thus, starting with an initial position q_0 and an initial momentum p_0 , the repeated solution of $\tilde{\varphi}_h$ gives the same discrete trajectory $\{q_n\}_{n=0}^N$ as the repeated solution of φ_h . The position-momentum form, as a one-step method, is usually easier to implement than the discrete Euler-Lagrange equations. And for most problems, initial conditions are more naturally prescribed via the position and momentum of the particle at a given point in time, (q_0, p_0) . If, however, only the position of the particle at two points in time, (q_0, q_1) , is known, the Euler-Lagrange equations are the more natural way of describing the dynamics.

This of course is just reflecting the difference in the Lagrangian and Hamiltonian point of view. For d degrees of freedom, the variational principle leads to d differential equations of second order. Hamilton's equations, on the other hand, are $2d$ differential equations of first order. Which form is more convenient to use largely depends on the problem at hand.

Example: Point Particle

Consider a particle with mass m , moving in some potential V . Its continuous Lagrangian is

$$L(q, \dot{q}) = \frac{1}{2} m \dot{q}^2 - V(q) \quad (7.35)$$

Approximated by the trapezoidal rule, the discrete Lagrangian reads

$$L_d^{\text{tr}}(q_n, q_{n+1}) = h \left[\frac{m}{2} \left(\frac{q_{n+1} - q_n}{h} \right)^2 - \frac{V(q_n) + V(q_{n+1})}{2} \right]. \quad (7.36)$$

Applying the discrete Euler-Lagrange equations (7.27) to this expression results in discrete equations of motion

$$m \frac{q_{n+1} - 2q_n + q_{n-1}}{h^2} = -\nabla V(q_n) \quad (7.37)$$

which clearly are a discrete version of Newton's second law

$$m\ddot{q} = -\nabla V = F. \quad (7.38)$$

For comparison, consider also the midpoint approximation

$$L_d^{\text{mp}}(q_n, q_{n+1}) = h \left[\frac{m}{2} \left(\frac{q_{n+1} - q_n}{h} \right)^2 - V\left(\frac{q_n + q_{n+1}}{2}\right) \right] \quad (7.39)$$

which leads to

$$m \frac{q_{n+1} - 2q_n + q_{n-1}}{h^2} = -\frac{1}{2} \left[\nabla V\left(\frac{q_{n-1} + q_n}{2}\right) + \nabla V\left(\frac{q_n + q_{n+1}}{2}\right) \right] \quad (7.40)$$

and thus a different discretisation of (7.38). The position-momentum form (7.33) of the trapezoidal Lagrangian (7.36) can be written as

$$\frac{q_{n+1} - q_n}{h} = \frac{1}{m} \left[p_n - \frac{h}{2} \nabla V(q_n) \right] \quad (7.41a)$$

$$\frac{p_{n+1} - p_n}{h} = -\frac{1}{2} \left[\nabla V(q_n) + \nabla V(q_{n+1}) \right] \quad (7.41b)$$

and the one of the midpoint Lagrangian (7.39) reads

$$\frac{q_{n+1} - q_n}{h} = \frac{1}{m} \left[p_n - \frac{h}{2} \nabla V\left(\frac{q_n + q_{n+1}}{2}\right) \right] \quad (7.42a)$$

$$\frac{p_{n+1} - p_n}{h} = -\nabla V\left(\frac{q_n + q_{n+1}}{2}\right). \quad (7.42b)$$

This bears a close resemblance of Hamilton's equations of motion, where the additional term in the first equations can be interpreted as extrapolating the momentum p_n to $t_{n+1/2}$. As already noted, it is not always so easy to solve (7.33a) for q_{n+1} , but in general this is an implicit equation.

7.4 Discrete Symplectic Form

As in the continuous case, the discrete one-form is obtained by computing the variation of the action for varying endpoints

$$\begin{aligned} d\mathcal{A}_d[q_d] \cdot v_d &= \sum_{n=0}^{N-1} [D_1 L_d(q_n, q_{n+1}) \cdot v_n + D_2 L_d(q_n, q_{n+1}) \cdot v_{n+1}] \\ &= \sum_{n=1}^{N-1} [D_1 L_d(q_n, q_{n+1}) + D_2 L_d(q_{n-1}, q_n)] \cdot v_n \\ &\quad + D_1 L_d(q_0, q_1) \cdot v_0 + D_2 L_d(q_{N-1}, q_N) \cdot v_N. \end{aligned} \quad (7.43)$$

The two latter terms originate from the variation at the boundaries. They form the discrete counterpart of the Lagrangian one-form. However, there are two boundary terms that define two distinct one-forms on $\mathcal{M} \times \mathcal{M}$,

$$\begin{aligned} \Theta_{L_d}^-(q_0, q_1) \cdot (v_0, v_1) &\equiv -D_1 L_d(q_0, q_1) \cdot v_0, \\ \Theta_{L_d}^+(q_{N-1}, q_N) \cdot (v_{N-1}, v_N) &\equiv D_2 L_d(q_{N-1}, q_N) \cdot v_N. \end{aligned} \quad (7.44)$$

In general, these one-forms are defined as

$$\begin{aligned} \Theta_{L_d}^-(q_n, q_{n+1}) &\equiv -D_1 L_d(q_n, q_{n+1}) dq_n, \\ \Theta_{L_d}^+(q_n, q_{n+1}) &\equiv D_2 L_d(q_n, q_{n+1}) dq_{n+1}. \end{aligned} \quad (7.45)$$

As $dL_d = \Theta_{L_d}^+ - \Theta_{L_d}^-$ and $d^2 L_d = 0$ one observes that

$$d\Theta_{L_d}^+ = d\Theta_{L_d}^- \quad (7.46)$$

such that the exterior derivative of both discrete one-forms defines the same *discrete Lagrangian two-form* or *discrete symplectic form*

$$\omega_{L_d} = d\Theta_{L_d}^+ = d\Theta_{L_d}^- = \frac{\partial^2 L_d(q_n, q_{n+1})}{\partial q_n \partial q_{n+1}} dq_n \wedge dq_{n+1} \quad (\text{no summation over } n). \quad (7.47)$$

Consider the exterior derivative of the discrete action (7.14). Upon insertion of the discrete Euler-Lagrange equations (7.27) it becomes

$$d\mathcal{A}_d = D_1 L_d(q_0, q_1) \cdot dq_0 + D_2 L_d(q_{N-1}, q_N) \cdot dq_N = \Theta_{L_d}^+(q_{N-1}, q_N) - \Theta_{L_d}^-(q_0, q_1). \quad (7.48)$$

On the right hand side we find the just defined Lagrangian one-forms (7.45). Taking the exterior derivative of (7.48) gives

$$\omega_{L_d}(q_0, q_1) = \omega_{L_d}(q_{N-1}, q_N), \quad (7.49)$$

where q_{N-1} and q_N are connected with q_0 and q_1 through the discrete Euler-Lagrange equations (7.27). Therefore, (7.49) implies that the discrete symplectic structure ω_{L_d} is preserved while the system advances from $t = 0$ to $t = Nh$ according to the discrete equations of motion (7.27). As the number of time steps N is arbitrary, the discrete symplectic form ω_{L_d} is preserved at all times of the simulation. Note that this does not automatically imply that the continuous symplectic structure ω_L is preserved under the discrete map φ_h .

7.5 Discrete Noether Theorem

The discrete Noether theorem, just as the continuous Noether theorem, draws the connection between symmetries of a discrete Lagrangian and quantities that are conserved by the discrete Euler-Lagrange equations or, equivalently, the discrete Lagrangian flow. The continuous theory translates straight forwardly to the discrete case. Therefore, we repeat just the important steps, translated to the discrete setting.

Consider a one parameter group of discrete curves $q_d^\epsilon = \{q_n^\epsilon\}_{n=0}^N$ with $q_n^\epsilon = \sigma^\epsilon(t_n, q_n, \epsilon)$ such that $q_n^0(q_n) = q_n$, i.e., $\sigma^0 = \text{id}$ (note that σ^ϵ is the same function as in the continuous case). The discrete Lagrangian L_d has a symmetry if it is invariant under this transformation

$$L_d(q_n^\epsilon, q_{n+1}^\epsilon) = L_d(q_n, q_{n+1}) \quad \text{for all } \epsilon \text{ and } n. \quad (7.50)$$

The generating vector field of such a symmetry transformation is

$$X_n = \left. \frac{\partial \sigma^\epsilon}{\partial \epsilon} \right|_{\epsilon=0} \quad (7.51)$$

such that

$$\left. \frac{d}{d\epsilon} L_d(q_n^\epsilon, q_{n+1}^\epsilon) \right|_{\epsilon=0} = D_1 L_d(q_n, q_{n+1}) \cdot X_n + D_2 L_d(q_n, q_{n+1}) \cdot X_{n+1}. \quad (7.52)$$

If $\{q_n\}_{n=0}^N$ solves the discrete Euler-Lagrange equations (7.27),

$$D_1 L_d(q_n, q_{n+1}) + D_2 L_d(q_{n-1}, q_n) = 0, \quad (7.53)$$

we can replace the first term on the right hand side of (7.52) to get

$$0 = -D_2 L_d(q_{n-1}, q_n) \cdot X_n + D_2 L_d(q_n, q_{n+1}) \cdot X_{n+1}. \quad (7.54)$$

This amounts to a discrete conservation law of the form

$$D_2 L_d(q_{n-1}, q_n) \cdot X_n = D_2 L_d(q_n, q_{n+1}) \cdot X_{n+1}. \quad (7.55)$$

It states that solutions $\{q_n\}_{n=0}^N$ of the discrete Euler-Lagrange equations preserve the components of the momentum $p_n = D_2 L_d(q_{n-1}, q_n)$ in direction X_n .

Free Point Particle

Consider a transformation that amounts to an infinitesimal spatial translation

$$q_n^\epsilon = q_n + \epsilon X. \quad (7.56)$$

The discrete Lagrangian is invariant under this transformation

$$L_d(q_n^\epsilon, q_{n+1}^\epsilon) = \frac{h}{2} \left(\frac{q_{n+1} + \epsilon X - q_n - \epsilon X}{h} \right)^2 = \frac{h}{2} \left(\frac{q_{n+1} - q_n}{h} \right)^2 = L_d(q_n, q_{n+1}), \quad (7.57)$$

such that the symmetry condition is trivially fulfilled

$$\left. \frac{d}{d\epsilon} L_d(q_n^\epsilon, q_{n+1}^\epsilon) \right|_{\epsilon=0} = 0. \quad (7.58)$$

The discrete conservation law following from the symmetry of the Lagrangian under spatial translation

$$\left(\frac{q_n - q_{n-1}}{h}\right) \cdot X = \left(\frac{q_{n+1} - q_n}{h}\right) \cdot X \quad (7.59)$$

amounts to the preservation of the discrete momentum in direction of X .

Energy

In continuous particle dynamics, the conservation of energy follows from translational symmetry of the Lagrangian with respect to time. In discrete particle dynamics, with a fixed timestep h , it is not possible to consider infinitesimal translations with respect to time. In the setting we described, it is therefore not possible to prove conservation of the discrete energy by applying Noether's theorem. Indeed, most often we find that energy is not conserved exactly, but only approximately, in that the energy error is bounded by some threshold value. This behaviour is typical for symplectic methods (see e.g. Hairer, Lubich, and Wanner [31] and references therein). Nevertheless, it is possible to achieve and prove exact energy conservation by making the timestep h a dynamical variable. It is thereby determined by the variational principle, such that energy is conserved exactly [42]. And in the Noether theorem, infinitesimal transformations of time can be considered as well.

However, we do not follow this path. Still we are interested in the energy conserving properties of our variational integrators. We therefore "read" the expression for the discrete energy from the Lagrangian. In the case of the free particle (and in most other cases) the Hamiltonian is an explicit part of the Lagrangian, such that its discrete counterpart follows directly from the discretisation of the Lagrangian.

7.6 Variational Error Analysis

In this section we want to show how the error of a variational integrator can be deduced from the error of the discrete Lagrangian. Let Φ_t^L denote the flow of the Euler-Lagrange equations of L and φ_h the flow of the discrete Euler-Lagrange equations of some discretisation L_d of L and $\tilde{\varphi}_h$ the flow of the corresponding discrete Hamiltonian map. Instead of considering how closely the trajectory of $\varphi_h^{L_d}$ matches the exact trajectory given by Φ_t^L , we consider how closely the discrete Lagrangian L_d matches the exact discrete Lagrangian L_d^e given by the action, namely

$$L_d^e(q_n, q_{n+1}) = \int_{t_n}^{t_{n+1}} L(q_{n,n+1}(t), \dot{q}_{n,n+1}(t)) dt, \quad (7.60)$$

where $q_{n,n+1}(t)$ is the solution of the Euler-Lagrange equations satisfying $q_{n,n+1}(t_n) = q_n$ and $q_{n,n+1}(t_{n+1}) = q_{n+1}$.

Definition 7.1. A discrete Lagrangian L_d is said to be of order r if there exists an open set $\mathcal{U}_v \subset \mathcal{T}\mathcal{M}$ and constants $C_v > 0$ and $h_v > 0$, so that

$$\|L_d(q_n, q_{n+1}) - L_d^e(q_n, q_{n+1})\| \leq C_v h^{r+1}, \quad (7.61)$$

for all solutions $q(t)$ of the Euler-Lagrange equations with initial conditions $(q, \dot{q}) \in \mathcal{U}_v$ and for all timesteps $h \leq h_v$.

Definition 7.2. The discrete fibre derivatives $\mathbb{F}^+ L_d$ and $\mathbb{F}^- L_d$ of a discrete Lagrangian L_d are said to be of order r if there exists an open set $\mathcal{U}_f \subset \mathbb{T}^* \mathcal{M}$ and constants $C_f > 0$ and $h_f > 0$, so that

$$\|\mathbb{F}^+ L_d(q_n, q_{n+1}) - \mathbb{F}^+ L_d^e(q_n, q_{n+1})\| \leq C_v h^{r+1}, \quad (7.62a)$$

$$\|\mathbb{F}^- L_d(q_n, q_{n+1}) - \mathbb{F}^- L_d^e(q_n, q_{n+1})\| \leq C_v h^{r+1}, \quad (7.62b)$$

for all solutions $q(t)$ of the Euler-Lagrange equations with initial conditions $(q, p) \in \mathcal{U}_v$ and for all timesteps $h \leq h_f$.

The orders of a discrete Lagrangian, its discrete Legendre transforms and its discrete Hamiltonian map are tightly related.

Theorem 7.3. Given a regular Lagrangian L and corresponding Hamiltonian H , the following statements are equivalent for a discrete Lagrangian L_d :

- (a) The discrete Hamiltonian map $\tilde{\varphi}_h$ for L_d is of order r .
- (b) The discrete Legendre transforms $\mathbb{F}^+ L_d$ and $\mathbb{F}^- L_d$ of L_d are of order r .
- (c) L_d is equivalent to a discrete Lagrangian \bar{L}_d of order r , that is

$$L_d = \bar{L}_d + f(h). \quad (7.63)$$

Proof. See Marsden and West [56, p.400-401]. □

The order of a discrete Lagrangian L_d can be calculated by expanding the expression for $L_d(q(0), q(h))$ in a Taylor series in h and by comparing this to the same expansion $L_d^e(q(0), q(h))$ of the exact Lagrangian. The first two terms of the expansion of the exact Lagrangian give

$$L_d^e(q(0), q(h)) = hL(q(0), \dot{q}(0)) + \frac{1}{2}h^2 \left(\frac{\partial L}{\partial \mathbf{x}}(q(0), \dot{q}(0)) \cdot \dot{q}(0) + \frac{\partial L}{\partial \mathbf{v}}(q(0), \dot{q}(0)) \cdot \ddot{q}(0) \right) + \mathcal{O}(h^3). \quad (7.64)$$

Higher derivatives of $q(t)$ are determined by the Euler-Lagrange equations. Consider a family of discrete Lagrangians

$$L_d^\alpha(q_n, q_{n+1}) = hL\left((1-\alpha)q_n + \alpha q_{n+1}, \frac{q_{n+1} - q_n}{h}\right), \quad (7.65)$$

with $\alpha \in [0, 1]$. The expansion of L_d^α is

$$L_d^\alpha(q(0), q(h)) = hL(q(0), \dot{q}(0)) + \frac{1}{2}h^2 \left(2\alpha \frac{\partial L}{\partial \mathbf{x}}(q(0), \dot{q}(0)) \cdot \dot{q}(0) + \frac{\partial L}{\partial \mathbf{v}}(q(0), \dot{q}(0)) \cdot \ddot{q}(0) \right) + \mathcal{O}(h^3). \quad (7.66)$$

Comparing this to the expansion for the exact discrete Lagrangian shows that the method is second-order if and only if $\alpha = 1/2$, otherwise it is only consistent.

For the Lagrangian

$$L(q(t), \dot{q}(t)) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q), \quad (7.67)$$

the Hamiltonian vector field is computed as

$$\dot{q} = M^{-1}p, \quad \dot{p} = -\nabla V(q), \quad (7.68)$$

so that the flow $(q(h), p(h)) = \tilde{\Phi}_h(q(0), p(0))$ has the expansion

$$q(h) = q(0) + hM^{-1}p(0) - \frac{1}{2}h^2M^{-1}\nabla V(q(0)) + \mathcal{O}(h^3), \quad (7.69)$$

$$p(h) = p(0) - h\nabla V(q(0)) - \frac{1}{2}h^2\nabla^2 V(q(0))M^{-1}p(0) + \mathcal{O}(h^3). \quad (7.70)$$

The discrete Hamiltonian map $\tilde{\varphi}_h$ is implicitly defined by

$$\frac{q_{n+1} - q_n}{h} = M^{-1}(\alpha p_n + (1 - \alpha)p_{n+1}), \quad (7.71a)$$

$$\frac{p_{n+1} - p_n}{h} = -\nabla V((1 - \alpha)q_n + \alpha q_{n+1}). \quad (7.71b)$$

Expanding the first step in h gives

$$q_1 = q_0 + hM^{-1}p_0 - (1 - \alpha)h^2M^{-1}\nabla V(q_0) + \mathcal{O}(h^3), \quad (7.72a)$$

$$p_1 = p_0 - h\nabla V(q_0) - \alpha h^2\nabla^2 V(q_0)M^{-1}p_0 + \mathcal{O}(h^3). \quad (7.72b)$$

Comparing this to the continuous flow $\tilde{\Phi}_h$ we see that the method is second order if and only if $\alpha = 1/2$, and otherwise it is only consistent. Thus the local error and the error of the discrete Lagrangian agree.

7.7 Discrete Phasespace Action Principle

The simplest discretisations of the phasespace action,

$$\mathcal{A}[q(t), p(t)] = \int_{t_1}^{t_2} [\langle p, \dot{q} \rangle - H(q, p)] dt, \quad (7.73)$$

follows from discretising the trajectory $q(t)$ between t_n and t_{n+1} by linear interpolation between q_n and q_{n+1} , i.e.,

$$q_h(t)|_{[t_n, t_{n+1}]} = q_n \frac{t_{n+1} - t}{t_{n+1} - t_n} + q_{n+1} \frac{t - t_n}{t_{n+1} - t_n}, \quad (7.74)$$

and $p(t)$ as piecewise constant, that is

$$p_h(t)|_{[t_n, t_{n+1}]} = p_{n+1} \quad \text{and} \quad p_h(t)|_{[t_n, t_{n+1}]} = p_n, \quad (7.75)$$

respectively. We obtain two possible discretisations of the action by using Riemann quadrature, either from the left, $c_1 = 0$, or from the right, $c_1 = h$,

$$\mathcal{A}_d^-[q_d, p_d] = \sum_{n=0}^{N-1} \left[p_{n+1} \frac{q_{n+1} - q_n}{h} - H(q_n, p_{n+1}) \right], \quad (7.76a)$$

$$\mathcal{A}_d^+[q_d, p_d] = \sum_{n=0}^{N-1} \left[p_n \frac{q_{n+1} - q_n}{h} - H(q_{n+1}, p_n) \right]. \quad (7.76b)$$

Computing variations, we obtain

$$\begin{aligned} \mathcal{A}_d^-[q_d, p_d] &= \sum_{n=0}^{N-1} \left[-\frac{p_{n+1} - p_n}{h} - \frac{\partial H}{\partial x}(q_n, p_{n+1}) \right] \cdot \delta q_n \\ &\quad + \sum_{n=0}^{N-1} \left[\frac{q_{n+1} - q_n}{h} - \frac{\partial H}{\partial p}(q_{n+1}, p_n) \right] \cdot \delta p_{n+1} = 0. \end{aligned} \quad (7.77)$$

and

$$\begin{aligned} \delta \mathcal{A}_d^+[q_d, p_d] = \sum_{n=0}^{N-1} \left[-\frac{p_{n+1} - p_n}{h} - \frac{\partial H}{\partial x}(q_{n+1}, p_n) \right] \cdot \delta q_{n+1} \\ + \sum_{n=0}^{N-1} \left[\frac{q_{n+1} - q_n}{h} - \frac{\partial H}{\partial p}(q_{n+1}, p_n) \right] \cdot \delta p_n = 0, \end{aligned} \quad (7.78)$$

Requiring the variations of the discrete actions to vanish, $\delta \mathcal{A}_d^- = 0$ and $\delta \mathcal{A}_d^+ = 0$, where in the first case we assume that $\delta q_N = 0$ and $\delta p_0 = 0$, while in the second case we assume that $\delta q_0 = 0$ and $\delta p_N = 0$, we obtain

$$\frac{q_{n+1} - q_n}{h} = \frac{\partial H}{\partial p}(q_n, p_{n+1}), \quad \frac{p_{n+1} - p_n}{h} = -\frac{\partial H}{\partial x}(q_n, p_{n+1}), \quad (7.79)$$

and

$$\frac{q_{n+1} - q_n}{h} = \frac{\partial H}{\partial p}(q_{n+1}, p_n), \quad \frac{p_{n+1} - p_n}{h} = -\frac{\partial H}{\partial x}(q_{n+1}, p_n), \quad (7.80)$$

which are the symplectic Euler-B and symplectic Euler-A methods, respectively.

7.8 Higher Order Variational Integrators by Composition

Similar to symplectic methods, the composition of a one-step variational integrator $\tilde{\varphi}$ with different step sizes is a simple method of obtaining higher order schemes. For variational integrators, however, there are some interesting additional results. We will show that a variational integrator is self-adjoint and thereby symmetric if its discrete Lagrangian is self-adjoint, a condition that is easily checked. Also, the composition can already be implemented at the level of the Lagrangian such that the composition of a variational integrator is itself a variational integrator. This has consequences for the discrete Noether theorem and the discrete conservation laws.

7.8.1 Adjoint of a Method and Adjoint Lagrangians

In this subsection, we show that a variational integrator is symmetric if its Lagrangian is self-adjoint. The adjoint $\tilde{\varphi}^*$ of a method $\tilde{\varphi}$ is defined as

$$(\tilde{\varphi}^*(h)) \circ (\tilde{\varphi}(-h)) = \text{id}. \quad (7.81)$$

A method $\tilde{\varphi}$ is self-adjoint if $\tilde{\varphi}^* = \tilde{\varphi}$, therefore a self-adjoint method is also symmetric. We would like to establish a condition of the discrete Lagrangian that tells us if the resulting method is self-adjoint or not. We therefore define the adjoint Lagrangian L_d^* of a discrete Lagrangian L_d as

$$L_d^*(q_n, q_{n+1}, h) \equiv -L_d(q_{n+1}, q_n, -h). \quad (7.82)$$

Hence the Lagrangian L_d is self-adjoint if

$$L_d(q_n, q_{n+1}, h) = -L_d(q_{n+1}, q_n, -h). \quad (7.83)$$

We want to show that if a discrete Lagrangian is self-adjoint so is the resulting method. We start by establishing that adjoint Lagrangians admit adjoint methods, i.e., if $\tilde{\varphi}$ is the Hamiltonian map resulting from L_d and $\tilde{\varphi}^*$ is the map resulting from L_d^* then $\tilde{\varphi}^* = \tilde{\varphi}^*$. In position momentum-form (7.33), the map $\tilde{\varphi}$ is defined as

$$\tilde{\varphi} : \begin{cases} p_n &= -D_1 L_d(q_n, q_{n+1}, h), \\ p_{n+1} &= D_2 L_d(q_n, q_{n+1}, h). \end{cases} \quad (7.84)$$

Its adjoint method $\tilde{\varphi}^*(h) = (\tilde{\varphi}(-h))^{-1}$ is the map

$$\tilde{\varphi}^* : \begin{cases} p_n &= D_2 L_d(q_{n+1}, q_n, -h), \\ p_{n+1} &= -D_1 L_d(q_{n+1}, q_n, -h). \end{cases} \quad (7.85)$$

And the map $\tilde{\varphi}^*$ corresponding to the adjoint Lagrangian (7.82) is

$$\tilde{\varphi}^* : \begin{cases} p_n &= -D_1 L_d^*(q_n, q_{n+1}, h), \\ p_{n+1} &= D_2 L_d^*(q_n, q_{n+1}, h). \end{cases} \quad (7.86)$$

Computing the derivatives of the definition of the adjoint Lagrangian (7.82)

$$\begin{aligned} D_1 L_d^*(q_n, q_{n+1}, h) &= -D_2 L_d(q_{n+1}, q_n, -h), \\ -D_2 L_d^*(q_n, q_{n+1}, h) &= D_1 L_d(q_{n+1}, q_n, -h), \end{aligned} \quad (7.87)$$

establishes the equality of (7.85) and (7.86), i.e., if two Lagrangians are adjoint so are the resulting methods. Computing the derivatives of the definition of the self-adjoint Lagrangian (7.83),

$$D_1 L_d(q_n, q_{n+1}, h) = -D_2 L_d(q_{n+1}, q_n, -h), \quad (7.88a)$$

$$-D_2 L_d(q_n, q_{n+1}, h) = D_1 L_d(q_{n+1}, q_n, -h), \quad (7.88b)$$

establishes the equality of (7.84) and (7.85), i.e., if the Lagrangian is self-adjoint so is the resulting method. We have thereby obtained a condition for symmetry of a variational integrator that can easily be checked.

7.8.2 Composite Discrete Lagrangians

The methods resulting from the application of symplectic composition schemes to variational integrators can all be derived as Euler-Lagrange equations from a composite discrete Lagrangian. Considering a method

$$\hat{\varphi}_h = \tilde{\varphi}_{\gamma_s h} \circ \dots \circ \tilde{\varphi}_{\gamma_i h} \circ \dots \circ \tilde{\varphi}_{\gamma_1 h}, \quad (7.89)$$

with s substeps $Q_{n,i}$ located at $t_{n,i} = t_n + \gamma_i h$, the corresponding composite discrete Lagrangian can be written as

$$\hat{L}_d(Q_{n,1}, \dots, Q_{n,s}) = \sum_{i=1}^s L_d(Q_{n,i-1}, Q_{n,i}, \gamma_i h), \quad (7.90)$$

where we identify $q_n = Q_{n,1}$ and $q_{n+1} = Q_{n,s}$ such that $Q_{n,s} = Q_{n+1,1}$. The discrete action becomes

$$\mathcal{A}_d(\{q_n = Q_{n,1}, \dots, Q_{n,s} = q_{n+1}\}_{n=0}^{N-1}) = \sum_{n=0}^{N-1} \hat{L}_d(Q_{n,1}, \dots, Q_{n,s}), \quad (7.91)$$

and we obtain discrete Euler-Lagrange equations

$$D_2 L_d(Q_{n-1,s-1}, Q_{n-1,s}, \gamma_s h) + D_1 L_d(Q_{n,1}, Q_{n,2}, \gamma_1 h) = 0 \quad (7.92a)$$

$$\vdots$$

$$D_2 L_d(Q_{n,i-1}, Q_{n,i}, \gamma_i h) + D_1 L_d(Q_{n,i}, Q_{n,i+1}, \gamma_{i+1} h) = 0 \quad (7.92b)$$

$$\vdots$$

$$D_2 L_d(Q_{n,s-1}, Q_{n,s}, \gamma_s h) + D_1 L_d(Q_{n+1,1}, Q_{n+1,2}, \gamma_1 h) = 0. \quad (7.92c)$$

The maps $\tilde{\varphi}_{\gamma_i h}$ in the composition method (7.89) can therefore be written as

$$\tilde{\varphi}_{\gamma_i h} : (Q_{n,i-1}, P_{n,i-1}) \mapsto (Q_{n,i}, P_{n,i}), \quad (7.93)$$

with

$$P_{n,i-1} = -D_1 L_d(Q_{n,i-1}, Q_{n,i}, \gamma_i h), \quad (7.94a)$$

$$P_{n,i} = D_2 L_d(Q_{n,i-1}, Q_{n,i}, \gamma_i h). \quad (7.94b)$$

The existence of a composite Lagrangian \hat{L}_d corresponding to a composite method $\hat{\varphi}$ is important in the analysis of conserved quantities. The discrete Noether theorem has to be applied to the composite Lagrangian to determine the quantities that are discretely conserved. Further, it cannot be expected that the error of the energy corresponding to the discrete Lagrangian L_d , which is used to build the composition scheme, scales with the order of the composition scheme.

7.8.3 Discrete Conservation Laws of Composite Lagrangians

Special care has to be taken when applying the discrete Noether theorem to composite discrete Lagrangians (7.90), which in general can be written as

$$\hat{L}_d(Q_{n,1}, \dots, Q_{n,s}) = \sum_{i=1}^s L_d^i(Q_{n,i-1}, Q_{n,i}, \gamma_i h), \quad (7.95)$$

where we allow the L_d^i to be different from one another. Here, \hat{L}_d might have different discrete expressions of the conserved momenta than the L_d^i . And it might even have different conservational properties, i.e., not all conserved momenta of \hat{L}_d might be conserved by the L_d^i or vice versa. Therefore the discrete Noether theorem (7.55) has to be applied to \hat{L}_d .

Similarly, the discrete expression for the energy can be different for \hat{L}_d and each of the L_d^i . To clarify this, let us look at an example. Consider the midpoint Lagrangian (7.17),

$$L_d^{\text{mp}}(q_n, q_{n+1}) = h L\left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{h}\right), \quad (7.96)$$

and the fourth order, three step composition method,

$$\hat{\varphi}_h = \tilde{\varphi}_{\gamma h} \circ \tilde{\varphi}_{(1-2\gamma)h} \circ \tilde{\varphi}_{\gamma h} \quad \text{with} \quad \gamma = (2 - 2^{1/(r+1)})^{-1}. \quad (7.97)$$

Assuming that the Lagrangian L is of the form

$$L(q, \dot{q}) = \dot{q}^T M \dot{q} - H(q, \dot{q}), \quad (7.98)$$

the discrete Hamiltonian corresponds to

$$H_d = h H\left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{h}\right), \quad (7.99)$$

such that the discrete Hamiltonian of the composite Lagrangian is given by

$$\begin{aligned} \hat{H}_d(Q_{n,1}, Q_{n,2}, Q_{n,3}, Q_{n,4}) = h & \left[\gamma H\left(\frac{Q_{n,1} + Q_{n,2}}{2}, \frac{Q_{n,2} - Q_{n,1}}{h}\right) \right. \\ & \left. + (1 - 2\gamma) H\left(\frac{Q_{n,2} + Q_{n,3}}{2}, \frac{Q_{n,3} - Q_{n,2}}{h}\right) + \gamma H\left(\frac{Q_{n,3} + Q_{n,4}}{2}, \frac{Q_{n,4} - Q_{n,3}}{h}\right) \right], \end{aligned} \quad (7.100)$$

where $Q_{n,1} = q_n$ and $Q_{n,4} = q_{n+1}$. Only the error of this composite Hamiltonian is guaranteed to scale with the order r of the scheme. That might at first seem surprising, as symplectic methods are supposed to conserve a direct discretisation of the continuous Hamiltonian to at least order r , i.e.,

$$H(q_N, p_N) = H(q_0, p_0) + \mathcal{O}(h^r), \quad (7.101)$$

for exponentially long time intervals $nh \leq e^{h_0/2h}$ with some constant h_0 . However, in the proof of this relation we assumed that the discrete flow map $\hat{\varphi}_h$ preserves the continuous symplectic form Ω . However, for general variational integrators we have only proved that the discrete symplectic form Ω_d is preserved. We can therefore not assume that this result translates directly. What we can always assume (for conservative systems) is that there exists a discrete energy that is preserved to the order of the scheme, and in the case of the composition schemes this is an expression analogous to (7.100).

7.9 Variational Runge-Kutta Methods

Another set of integrators of arbitrary high order are Runge-Kutta methods. Symplectic-partitioned Runge-Kutta integrators have been shown to be variational integrators [56, 31]. Here, the discrete Lagrangian has s internal points (or stages) located at $t_n + hc_i$ with weights b_i which are all non-zero and sum up to one,

$$L_d(q_n, q_{n+1}) = h \sum_{i=1}^s b_i L(Q_{n,i}, \dot{Q}_{n,i}). \quad (7.102)$$

The internal stages $Q_{n,i} \approx q(t_n + hc_i)$ are given by

$$Q_{n,i} = q_n + h \sum_{j=1}^s a_{ij} \dot{Q}_{n,j}. \quad (7.103)$$

In contrast to the composition methods, we do not require $c_1 = 0$ and $c_s = 1$. Instead the discrete action is extremised under the constraints

$$q_{n+1} = q_n + h \sum_{i=1}^s b_i \dot{Q}_{n,i}, \quad (7.104)$$

which we add to the action with the Lagrange multiplier λ_{n+1} , so that we can write

$$\mathcal{A}_d = \sum_{n=1}^{N-1} \left[h \sum_{i=1}^s b_i L(Q_{n,i}, \dot{Q}_{n,i}) + \lambda_{n+1} \cdot \left(q_{n+1} - q_n - h \sum_{i=1}^s b_i \dot{Q}_{n,i} \right) \right]. \quad (7.105)$$

Computing variations of the action leads to

$$\begin{aligned} \delta \mathcal{A}_d = & \sum_{n=1}^{N-1} \left[h \sum_{i=1}^s h b_i a_{ij} \frac{\partial L}{\partial X}(Q_{n,i}, \dot{Q}_{n,i}) + h b_j \frac{\partial L}{\partial V}(Q_{n,j}, \dot{Q}_{n,j}) - h b_j \lambda_{n+1} \right] \cdot \delta \dot{Q}_{n,j} \\ & + \sum_{n=1}^{N-1} \left[h \sum_{i=1}^s b_i \frac{\partial L}{\partial X}(Q_{n,i}, \dot{Q}_{n,i}) - \lambda_{n+1} + \lambda_n \right] \cdot \delta q_n \\ & + \sum_{n=1}^{N-1} \left[q_{n+1} - q_n - h \sum_{i=1}^s b_i \dot{Q}_{n,i} \right] \cdot \delta \lambda_{n+1} = 0. \end{aligned} \quad (7.106)$$

We define

$$\dot{P}_{n,i} = \frac{\partial L}{\partial X}(Q_{n,i}, \dot{Q}_{n,i}) \quad \text{and} \quad P_{n,i} = \frac{\partial L}{\partial V}(Q_{n,i}, \dot{Q}_{n,i}), \quad (7.107)$$

so that the terms of (7.106) which are multiplying $\delta \dot{Q}_{n,j}$ become

$$P_{n,j} = \lambda_{n+1} - h \sum_{i=1}^s \frac{b_i a_{ij}}{b_j} \dot{P}_{n,i}. \quad (7.108)$$

The terms of (7.106) which are multiplying δq_n become

$$\lambda_{n+1} = \lambda_n + h \sum_{i=1}^s b_i \dot{P}_{n,i}. \quad (7.109)$$

Similar to (7.33), we can define

$$p_n = -D_1 L_d(q_n, q_{n+1}) = \lambda_{n+1} - h \sum_{i=1}^s b_i \dot{P}_{n,i}, \quad (7.110a)$$

$$p_{n+1} = D_2 L_d(q_n, q_{n+1}) = \lambda_{n+1}, \quad (7.110b)$$

so that by inserting (7.110b) into (7.110a) we get

$$p_{n+1} = p_n + h \sum_{i=1}^s v_i \dot{P}_{n,i}, \quad (7.111)$$

which states that the second symplecticity condition ($b_i = \bar{b}_i$) is automatically satisfied. Insert (7.110a) into (7.108) to get

$$P_{n,j} = p_n + h \sum_{i=1}^s \bar{a}_{ij} \dot{P}_{n,i}, \quad (7.112)$$

with

$$\bar{a}_{ij} = b_j - b_j a_{ji} / b_i, \quad (7.113)$$

such that the first symplecticity condition is also satisfied. In summary, we obtain the variational-partitioned Runge-Kutta integrator

$$P_{n,i} = \frac{\partial L}{\partial V}(Q_{n,i}, \dot{Q}_{n,i}), \quad Q_{n,i} = q_n + h \sum_{j=1}^s a_{ij} \dot{Q}_{n,j}, \quad q_{n+1} = q_n + h \sum_{i=1}^s b_i \dot{Q}_{n,i}, \quad (7.114a)$$

$$\dot{P}_{k,i} = \frac{\partial L}{\partial X}(Q_{n,i}, \dot{Q}_{n,i}), \quad P_{n,j} = p_n + h \sum_{i=1}^s \bar{a}_{ij} \dot{P}_{n,i}, \quad p_{n+1} = p_n + h \sum_{i=1}^s b_i \dot{P}_{n,i}. \quad (7.114b)$$

If the fibre derivative is invertible, an equivalent set of equations can be obtained by applying

$$\dot{Q}_{n,i} = \frac{\partial H}{\partial p}(Q_{n,i}, P_{n,i}), \quad \dot{P}_{n,i} = -\frac{\partial H}{\partial x}(Q_{n,i}, P_{n,i}), \quad (7.115)$$

to the Hamiltonian $H(q, p)$ obtained via the Legendre transform. The interested reader can find more details on this in Hairer, Lubich, and Wanner [31] and references therein.

Remark 7.4. *Some words of caution are in order. The above derivation works well, if all discrete velocities $\dot{Q}_{n,i}$ are independent of one another. This is the case e.g. for Gauss-Legendre discretisations but not for Gauss-Lobatto discretisations (see [64] for details). If the velocities are not independent, this has to be accounted for when computing the variations. In order to avoid such subtleties, which are easily overlooked, it is recommendable to start the discretisation of the action from a more fundamental point of view, by approximating the function spaces of the trajectories, which leads us to the Galerkin variational integrators of the next section.*

Another approach that always works is to use the discretisation (7.102) of the Lagrangian, drop the constraint in the action (7.105), and compute the position-momentum form (7.33) of the variational integrator.

7.10 Galerkin Variational Integrators

From the considerations in the previous section, it follows that certain partitioned Runge-Kutta methods are symplectic due to being variational, but it does not become clear, how to choose the coefficients a_{ij} and weights b_i in a systematic way.

In the following, we first present the Galerkin framework for variational integrators [49, 50, 12, 65, 13, 64] where the space of curves \mathcal{Q} that connect two points in \mathcal{M} is approximated by a finite-dimensional subspace (Galerkin integrators of 0th kind). We use Lagrange polynomials to approximate the trajectories albeit other choices are possible. Alternatively, we can approximate the generalised velocities (Galerkin integrators of 1st kind), which leads us to variational-partitioned Runge-Kutta methods. Even though, in some cases correspondences between integrators of 0th kind and integrators of 1st kind might be found, in general they are different.

In our treatment we distinguish between integer timesteps, which are the coordinates q_n at time t_n , and internal stages (nodes), which are the coordinates $Q_{n,i}$ located between two integer timesteps q_n and q_{n+1} at consecutive points in time t_n and t_{n+1} . In all of the following we assume that the timestep h is constant.

In the discrete variational principle, we have to consider variations at both, the integer timesteps and the internal stages. For Galerkin integrators of 0th kind, the coordinates $Q_{n,i}$ are varied, whereas for the Galerkin integrators of 1st kind, the velocities $\dot{Q}_{n,i}$ are varied. So the independent variables are $(q_n, Q_{n,i})$ and $(q_n, \dot{Q}_{n,i})$, respectively.

7.10.1 Space of Discrete Trajectories

In order to construct the discrete space of curves from q_0 to q_N ,

$$\mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N) = \{q_d : \{t_n\}_{n=0}^N \rightarrow \mathcal{M} \mid q_d(t_0) = q_0, q_d(t_N) = q_N\} \subset \mathcal{Q}_d(\mathcal{M}), \quad (7.116)$$

we will construct a finite-dimensional subspace of

$$\mathcal{Q}(q_0, q_N, [0, T]) = \{q : [0, T] \rightarrow \mathcal{M} \mid q(0) = q_0, q(T) = q_N\} \subset \mathcal{Q}(\mathcal{M}). \quad (7.117)$$

The subspace $\mathcal{Q}_h(q_0, q_N, [0, T])$ is defined by

$$\mathcal{Q}_h(q_0, q_N, [0, T]) = \{q_h : [0, T] \rightarrow \mathcal{M} \mid q_h|_{[t_n, t_{n+1}]} \in \mathbb{P}_s([t_n, t_{n+1}]), q_h \in C^0([0, T])\}, \quad (7.118)$$

where $\mathbb{P}_s([t_n, t_{n+1}])$ is the space of polynomials of degree s in the interval $[t_n, t_{n+1}] \subset [0, T]$. We see that $\mathcal{Q}_h(q_0, q_N, [0, T]) \subset \mathcal{Q}(q_0, q_N, [0, T])$. In order for $\mathcal{Q}_h(q_0, q_N, [0, T])$ to be an instance of $\mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N)$ we have to require in addition to the definition (7.118) that on the sequence $\{t_n\}_{n=0}^N$, the curves q_h in $\mathcal{Q}_h(q_0, q_N, [0, T])$ satisfy

$$q_h|_{[t_n, t_{n+1}]}(t_n) = q_n \quad \text{and} \quad q_h|_{[t_n, t_{n+1}]}(t_{n+1}) = q_{n+1}, \quad (7.119)$$

where q_n are the points of the discrete trajectories $q_d = \{q_n\}_{n=0}^N$. However, it is often more convenient to enforce these continuity constraints weakly in the action rather than building them into the spaces, which implies dropping the condition $q_h \in C^0([0, T])$ in (7.118). This in turn means that the whole of $\mathcal{Q}_h(q_0, q_N, [0, T])$ is not a subspace of $\mathcal{Q}(q_0, q_N, [0, T])$ anymore.

7.10.2 Piecewise Polynomials

A basis of $\mathcal{Q}_h(q_0, q_N, [0, T])$ can easily be constructed by combining bases of $\mathbb{P}_s([t_n, t_{n+1}])$, e.g., using Lagrange polynomials. We start by specifying the collocation times of the internal stages. Select a set of s points c_i with $0 \leq c_i \leq 1$, which are the nodes of the basis functions. Therefore the basis is built by s functions. The internal stages are then located at $t_{n,i} = t_n + hc_i$, such that

$$t_n \leq t_{n,1} < \dots < t_{n,s} \leq t_{n+1}, \quad (7.120)$$

and we have

$$Q_{n,i} \approx q(t_{n,i}). \quad (7.121)$$

We will only be concerned with Lagrange polynomials. The j -th Lagrange polynomial of order s is defined by

$$l^{s,i}(\tau) = \prod_{\substack{1 \leq j \leq s, \\ j \neq i}} \frac{\tau - c_j}{c_i - c_j}. \quad (7.122)$$

The c_i are often chosen to be the collocation points of some quadrature rule (e.g., Gauß-Legendre or Gauß-Chebyshev points). Within each subinterval between two consecutive timesteps, t_n and t_{n+1} , the same Lagrange basis is used, namely

$$\text{span} \{ \varphi_n^{s,m}(t) \mid 1 \leq m \leq s \}, \quad (7.123)$$

with

$$\varphi_n^{s,m}(t) = \begin{cases} l^{s,m}((t - t_n)/(t_{n+1} - t_n)), & t_n \leq t \leq t_{n+1}, \\ 0, & \text{else.} \end{cases} \quad (7.124)$$

It suffices to specify the basis for one subinterval $[t_n, t_{n+1}]$ and then replicate this basis for all subintervals, so that the finite-dimensional subspace of $\mathcal{Q}(q_0, q_N, [0, T])$ is given by

$$\mathcal{Q}_h(q_0, q_N, [0, T]) = \left\{ q_h : [0, T] \rightarrow \mathcal{M} \mid q_h|_{[t_n, t_{n+1}]} \in \text{span} \{ \varphi_n^{s,m} \mid 1 \leq m \leq s \}, \right. \\ \left. q_h(0) = q_0, q_h(T) = q_N \right\}. \quad (7.125)$$

In order to obtain the discrete space of curves $\mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N)$ we have to add continuity constraints, connecting the polynomials in each interval with the nodal values q_n , that is

$$\mathcal{Q}_d(q_0, q_N, \{t_n\}_{n=0}^N) = \left\{ q_h \in \mathcal{Q}_h(q_0, q_N, [0, T]) \mid q_h|_{[t_n, t_{n+1}]}(t_n) = q_n, \right. \\ \left. q_h|_{[t_n, t_{n+1}]}(t_{n+1}) = q_{n+1} \right\}. \quad (7.126)$$

We project the trajectories of the particles onto a Lagrange basis in order to obtain the polynomial approximation of the trajectory in the interval $[t_n, t_{n+1}]$, i.e.,

$$q_h(t)|_{[t_n, t_{n+1}]} = \sum_{m=1}^s Q_{n,m} \varphi_n^{s,m}(t). \quad (7.127)$$

The particle velocities are then obtained by differentiating with respect to time,

$$\dot{q}_h(t)|_{[t_n, t_{n+1}]} = \sum_{m=1}^s Q_{n,m} \dot{\varphi}_n^{s,m}(t). \quad (7.128)$$

For $s = 2$, we obtain

$$q_h(t)|_{[t_n, t_{n+1}]} = Q_{n,1} \frac{t - t_{n+1}}{t_n - t_{n+1}} + Q_{n,2} \frac{t - t_n}{t_{n+1} - t_n}, \quad \dot{q}_h(t)|_{[t_n, t_{n+1}]} = \frac{Q_{n,2} - Q_{n,1}}{t_{n+1} - t_n}, \quad (7.129)$$

which is just linear interpolation for q and piecewise constant for \dot{q} .

7.10.3 Numerical Quadrature

In order to numerically compute the definite integral

$$F[q] = \int_{t_n}^{t_{n+1}} f(t, q(t)) dt, \quad (7.130)$$

we apply two levels of approximation. As $q(t)$ is unknown, we replace it with the piecewise polynomial approximation $q_h(t)$. Further, we introduce a quadrature formula in which f itself is approximated by a Lagrange polynomial, i.e.,

$$f_h(t, q(t)) = \sum_{i=1}^s \varphi_n^{s,i}(t) f(t_n + hc_i, q(t_n + hc_i)). \quad (7.131)$$

Together, this gives an approximation of the integral (7.130) as follows

$$F_h[q] = \int_{t_n}^{t_{n+1}} f_h(t, q_h(t)) dt = h \sum_{i=1}^s b_i f(t_n + hc_i, q_h(t_n + hc_i)), \quad (7.132)$$

where b_i are the weights or coefficients of the quadrature formula, given by

$$b_i = \frac{1}{h} \int_{t_n}^{t_{n+1}} \varphi_n^{s,i}(t) dt = \int_0^1 l^{s,i}(\tau) d\tau, \quad (7.133)$$

$h = t_{n+1} - t_n$ is the time step, and $q_h(t)|_{[t_n, t_{n+1}]}$ is some polynomial approximation to $q(t)$ in the interval $[t_n, t_{n+1}]$. We will focus on collocation methods where the nodes c_i of the quadrature

rule are also the nodes of the basis functions, so that for (7.127), we have $q_h(t_n + hc_i) = Q_{n,i}$. It follows that the discrete Lagrangian can be written as

$$L_d(q_n, q_{n+1}) = h \sum_{i=1}^s b_i L(Q_{n,i}, \dot{Q}_{n,i}). \quad (7.134)$$

Most often, we use Gauss-Legendre quadrature, where the nodes c_i are given by the roots of the Legendre polynomials. The Gauss quadrature rules with s nodes yield exact results when applied to polynomials of order up to $2s$.

7.10.4 Galerkin Variational Integrators of 0th Kind

In order, to write the discrete Lagrangian in the discrete action in a compact form, we define the nodal coefficients a_{ij} ,

$$a_{ij} = h \left. \frac{d\varphi_n^{s,j}}{dt} \right|_{t=t_n+hc_i} = \left. \frac{dl^{s,j}}{d\tau} \right|_{\tau=c_i}, \quad (7.135)$$

so that the velocities can be written as

$$\dot{Q}_{n,i} = \dot{q}_h(t_{n,i}) = \sum_{j=1}^s Q_{n,j} \dot{\varphi}_n^{s,j}(t_n + hc_i) = \frac{1}{h} \sum_{j=1}^s a_{ij} Q_{n,j}. \quad (7.136)$$

In order to complete the discrete action, we explicitly add the continuity constraint,

$$\begin{aligned} \mathcal{A}_d[q_d] = \sum_{n=0}^{N-1} \left[\sum_{i=1}^s b_i L(Q_{n,i}, \dot{Q}_{n,i}) + \lambda_n \cdot (q_h|_{[t_n, t_{n+1}]}(t_n) - q_n) \right. \\ \left. + \mu_{n+1} \cdot (q_h|_{[t_n, t_{n+1}]}(t_{n+1}) - q_{n+1}) \right], \end{aligned} \quad (7.137)$$

which ensures that the polynomials in neighbouring intervals, e.g., $[t_n, t_{n+1}]$ and $[t_{n+1}, t_{n+2}]$, have the same value at integer timesteps, e.g., t_{n+1} .

7.10.5 Galerkin Variational Integrators of 1st Kind

For the Galerkin variational integrators of 1st kind, we do not project the trajectories to a Lagrange basis but the velocities,

$$\dot{q}_h(t)|_{[t_n, t_{n+1}]} = \sum_{i=1}^s \dot{Q}_{n,i} \varphi_n^{s,i}(t), \quad (7.138)$$

where

$$\dot{Q}_{n,i} \approx \dot{q}(t_n + hc_i). \quad (7.139)$$

The coordinates at the internal stages are then obtained by integration, namely

$$Q_{n,i} = q_n + \int_{t_n}^{t_n+hc_i} \dot{q}_h(t) dt = q_n + \sum_{j=1}^s \dot{Q}_{n,j} \int_{t_n}^{t_n+hc_i} \varphi_n^{s,j}(t) dt, \quad (7.140)$$

which suggests to define nodal coefficients a_{ij} by

$$a_{ij} = \frac{1}{h} \int_{t_n}^{t_n+hc_i} \varphi_n^{s,j}(t) dt = \int_0^{c_i} l^{s,j}(\tau) d\tau, \quad (7.141)$$

so that

$$Q_{n,i} = q_n + h \sum_{j=1}^s a_{ij} \dot{Q}_{n,j}. \quad (7.142)$$

The coordinates at the next timestep are similarly obtained by

$$q_{n+1} = q_n + \int_{t_n}^{t_{n+1}} \dot{q}_h(t) dt = q_n + \sum_{j=1}^s \dot{Q}_{n,j} \int_{t_n}^{t_{n+1}} \varphi_n^{s,j}(t) dt = q_n + h \sum_{j=1}^s b_j \dot{Q}_{n,j}, \quad (7.143)$$

with the same weights b_j as before. As before, we need a continuity condition in the discrete action, which now corresponds to the update rule for the next timestep,

$$\mathcal{A}_d[q_d] = \sum_{n=0}^{N-1} \left[\sum_{i=1}^s b_i L(Q_{n,i}, \dot{Q}_{n,i}) + \lambda_{n+1} \cdot \left(q_{n+1} - q_n - \sum_{j=1}^s b_j \dot{Q}_{n,j} \right) \right], \quad (7.144)$$

which is the equivalent of the continuity constraint for the Galerkin integrators of 0th kind. This provides us with a systematic derivation of the discrete action (7.105).

8 Energy and Integral Preserving Integrators

Integral preserving integrators are numerical integration algorithms that preserve exactly one or more first integrals of a differential equation, e.g., energy, momentum or angular momentum. An ordinary differential equation $\dot{z} = f(z)$ with $z \in \mathbb{R}^d$ possesses s first integrals $I : \mathbb{R}^d \rightarrow \mathbb{R}^s$ if

$$\frac{d}{dt}I(z) = \nabla I(z)^T \dot{z} = \nabla I(z)^T f(z) = 0. \quad (8.1)$$

This implies that the solution $z(t)$ is constrained to the integral manifold (constraint submanifold)

$$\mathcal{N} = \{z \mid g(z) = 0\}, \quad (8.2)$$

where

$$g(z) = I(z) - I(z_0). \quad (8.3)$$

In order to construct integral preserving integrators we can proceed in various ways.

8.1 Projection Methods

Projection methods are the simplest integral-preserving methods. The standard projection method is defined as follows.

1. Compute $\tilde{z}_{n+1} = \varphi_h(z_n)$ by some integration method φ_h .
2. Project \tilde{z}_{n+1} onto \mathcal{N} to obtain $z_{n+1} \in \mathcal{N}$.

The projection step is usually obtained by minimising the Lagrange function

$$L(z_{n+1}, \lambda_{n+1}) = \frac{1}{2} \|z_{n+1} - \tilde{z}_{n+1}\|^2 - g(z_{n+1})^T \lambda_{n+1}, \quad (8.4)$$

where $\lambda_{n+1} = (\lambda_{n+1}^1, \dots, \lambda_{n+1}^s)^T$ represent Lagrange multipliers. Stationarity of the Lagrange function is then given by

$$\frac{\partial L}{\partial z_{n+1}} = 0 \quad \rightarrow \quad z_{n+1} = \tilde{z}_{n+1} + g'(z_{n+1})^T \lambda_{n+1}, \quad (8.5a)$$

$$\frac{\partial L}{\partial \lambda_{n+1}} = 0 \quad \rightarrow \quad g(z_{n+1}) = 0. \quad (8.5b)$$

The whole algorithm reads

$$\tilde{z}_{n+1} = \varphi_h(z_n), \quad (8.6a)$$

$$z_{n+1} = \tilde{z}_{n+1} + g'(z_{n+1})^T \lambda_{n+1}, \quad (8.6b)$$

$$g(z_{n+1}) = 0. \quad (8.6c)$$

For convenience, the argument of g' in the projection step is sometimes replaced with \tilde{z}_{n+1} , so that

$$z_{n+1} = \tilde{z}_{n+1} + g'(\tilde{z}_{n+1})^T \lambda_{n+1}, \quad g(z_{n+1}) = 0. \quad (8.7)$$

Since the projection step is now explicit, it can be substituted in the constraint in order to obtain implicit equations for the Lagrange multipliers λ_{n+1} . In order to obtain symmetric and reversible algorithms, a symmetric projection can be used. The total algorithm then reads

$$\tilde{z}_n = z_n + g'(z_n)^T \lambda_{n+1}, \quad (8.8a)$$

$$\tilde{z}_{n+1} = \varphi_h(\tilde{z}_n), \quad (8.8b)$$

$$z_{n+1} = \tilde{z}_{n+1} + g'(\tilde{z}_{n+1})^T \lambda_{n+1}, \quad (8.8c)$$

$$g(z_{n+1}) = 0, \quad (8.8d)$$

where it is important to use the same λ_{n+1} in both projection steps. Instead of z_n and z_{n+1} , one can also use $\frac{1}{2}(z_n + z_{n+1})$ in the arguments of g' in both of the projection steps.

8.2 Discrete Gradients

A second family of integral-preserving methods are so called discrete gradients, that is discrete analogues of the gradient of a function. Given an ODE $\dot{z} = f(z)$ with one or more first integrals $I(z)$, the ODE can be rewritten as a linear-gradient system. Then discrete gradients can be used to construct discrete approximations to the ODE which preserve the first integrals exactly. This method can be applied to all Hamiltonian, Poisson and gradient systems as well as to many dissipative systems.

In order to construct discrete gradients, we proceed in two steps.

1. Write the ODE in the form

$$\dot{z} = S(z) \nabla I(z), \quad (8.9)$$

where $S(z)$ is a skew-symmetric matrix. Such a matrix can always be found, e.g., in the form of

$$S(z) = \frac{1}{|\nabla I(z)|^2} \left(f(z) \nabla I(z)^T - \nabla I(z) f(z)^T \right). \quad (8.10)$$

Note that the matrix $S(z)$ is usually not uniquely defined.

2. Discretise (8.9) by

$$\frac{z_{n+1} - z_n}{h} = \tilde{S}(z_n, z_{n+1}) \bar{\nabla} I(z_n, z_{n+1}), \quad (8.11)$$

where $\tilde{S}(z_n, z_{n+1})$ is any skew-symmetric matrix that approaches $S(z)$ in the limit of $z_{n+1} \rightarrow z_n$ and $h \rightarrow 0$, and where $\bar{\nabla} I(z_n, z_{n+1})$ is a discrete gradient.

Definition 8.1. Given a differentiable function $I : \mathbb{R}^d \rightarrow \mathbb{R}$, a discrete gradient $\bar{\nabla} I(z_n, z_{n+1})$ is a vector valued continuous function of (z_n, z_{n+1}) satisfying

$$(z_{n+1} - z_n) \cdot \bar{\nabla} I(z_n, z_{n+1}) = I(z_{n+1}) - I(z_n), \quad (8.12a)$$

$$\bar{\nabla} I(z_n, z_n) = \nabla I(z_n). \quad (8.12b)$$

Various such discrete gradients are known.

1. Harten, Lax, and Leer [35] (average discrete gradient)

$$\bar{\nabla} I(z_n, z_{n+1}) = \int_0^1 \nabla I((1-\xi)z_n + \xi z_{n+1}) d\xi. \quad (8.13)$$

2. Gonzalez [28] (midpoint discrete gradient)

$$\bar{\nabla} I(z_n, z_{n+1}) = \nabla I(z_{n+1/2}) + (z_{n+1} - z_n) \frac{I(z_{n+1}) - I(z_n) - (z_{n+1} - z_n) \cdot \nabla I(z_{n+1/2})}{\|z_{n+1} - z_n\|^2}, \quad (8.14)$$

with $z_{n+1/2} = \frac{1}{2}(z_n + z_{n+1})$.

3. Itoh and Abe [39]

$$\bar{\nabla} I(z_n, z_{n+1})_i = \frac{I(z_n^{(i)}) - I(z_n^{(i-1)})}{z_{n+1}^i - z_n^i}, \quad (8.15)$$

where

$$z_n^{(i)} = (z_{n+1}^1, \dots, z_{n+1}^i, z_n^{i+1}, \dots, z_n^d). \quad (8.16)$$

Theorem 8.2. *Discrete gradients preserve first integrals.*

Proof. By definition, discrete gradients satisfy

$$I(z_{n+1}) - I(z_n) = \bar{\nabla} I(z_n, z_{n+1})^T (z_{n+1} - z_n), \quad (8.17)$$

so that when replacing $(z_{n+1} - z_n)$ with the discrete update rule,

$$z_{n+1} - z_n = h \tilde{S}(z_n, z_{n+1}) \bar{\nabla} I(z_n, z_{n+1}), \quad (8.18)$$

we get

$$I(z_{n+1}) - I(z_n) = h \bar{\nabla} I(z_n, z_{n+1})^T \tilde{S}(z_n, z_{n+1}) \bar{\nabla} I(z_n, z_{n+1}) = 0, \quad (8.19)$$

which vanishes as \tilde{S} is skew-symmetric. \square

All of the above discrete gradients as well as new families of discrete gradients can be constructed based on approximations of the trajectory in the interval $[t_n, t_{n+1}]$ and the following observation [52]. Suppose the scalar function $I : \mathbb{R}^d \rightarrow \mathbb{R}$ and $z_n, z_{n+1} \in \mathbb{R}^d$ are given. If some approximation $\tilde{I} : \mathbb{R}^d \rightarrow \mathbb{R}$ of I satisfies both

$$\tilde{I}(z_n) = I(z_n) \quad \text{and} \quad \tilde{I}(z_{n+1}) = I(z_{n+1}), \quad (8.20)$$

then for any discrete gradient $\bar{\nabla} \tilde{I}(z_n, z_{n+1})$ of \tilde{I} , such that

$$(z_{n+1} - z_n) \cdot \bar{\nabla} \tilde{I}(z_n, z_{n+1}) = \tilde{I}(z_{n+1}) - \tilde{I}(z_n), \quad (8.21)$$

we also have

$$(z_{n+1} - z_n) \cdot \bar{\nabla} \tilde{I}(z_n, z_{n+1}) = I(z_{n+1}) - I(z_n). \quad (8.22)$$

Assuming $z_{n+1} \neq z_n$, we therefore have (component-wise)

$$\bar{\nabla} \tilde{I}(z_n, z_{n+1}) = \frac{\tilde{I}(z_{n+1}) - \tilde{I}(z_n)}{z_{n+1} - z_n} = \frac{I(z_{n+1}) - I(z_n)}{z_{n+1} - z_n}, \quad (8.23)$$

such that when taking the limit $z_{n+1} \rightarrow z_n$ on both sides, we have

$$\bar{\nabla} \tilde{I}(z_n, z_n) = \nabla \tilde{I}(z_n) = \nabla I(z_n). \quad (8.24)$$

This implies that a discrete gradient for \tilde{I} yields a discrete gradient for I . Consider the average value of the gradient as given by Harten, Lax, and Leer as “prototypical” discrete gradient. Then the previous considerations lead to the following theorem.

Theorem 8.3. *For any given $I : \mathbb{R}^d \rightarrow \mathbb{R}$ and any two points x_n and x_{n+1} , we have that*

(i) *there exists an open set $\Omega \subset \mathbb{R}^d$, such that the straight line*

$$(1 - \xi)x_n + \xi x_{n+1}, \quad 0 \leq \xi \leq 1,$$

is contained wholly within Ω , and

(ii) *there exists $\tilde{I} : \Omega \rightarrow \mathbb{R}$, depending on x_n and x_{n+1} , satisfying*

$$\tilde{I}(z_n) = I(z_n) \quad \text{and} \quad \tilde{I}(z_{n+1}) = I(z_{n+1}). \quad (8.25)$$

Then a discrete gradient for I is given by

$$\bar{\nabla} I(x_n, x_{n+1}) = \int_0^1 \nabla \tilde{I}((1 - \xi)z_n + \xi z_{n+1}) d\xi. \quad (8.26)$$

Taking $\tilde{I}(x_n, x_{n+1}) = I(x_n, x_{n+1})$ for all (x_n, x_{n+1}) , we obtain the average value discrete gradient of Harten, Lax, and Leer [35]. The discrete gradients of Itoh and Abe [39] and Gonzalez [28] can also be obtained this way, albeit by slightly more complicate approximations \tilde{I} (see Mansfield and Quispel [52] for details).

Remark 8.4. *Integral preserving schemes can not only be used to exactly conserve integrals but also to exactly preserve the dissipation of an integral.*

Remark 8.5. *For the case of constant matrix S , the average discrete gradient method of Harten et al. reduces to the average vector field method [69],*

$$\frac{z_{n+1} - z_n}{h} = \int_0^1 f((1 - \xi)z_n + \xi z_{n+1}) d\xi. \quad (8.27)$$

Remark 8.6. *The generalisation of the discrete gradient method to PDEs is the so-called discrete variational derivative method [25].*

8.3 Generalised Collocation Methods

Higher order generalisations of average vector field methods and discrete gradients can be obtained by generalising collocation methods [30, 17]. The resulting integrators can be interpreted as Runge-Kutta methods with infinitely many stages.

As with classical collocation methods, we consider an s -point quadrature formula with nodes c_i . Denote the j -th Lagrange polynomial of order s by

$$l^{s,i}(\tau) = \prod_{\substack{1 \leq j \leq s, \\ j \neq i}} \frac{\tau - c_j}{c_i - c_j}, \quad (8.28)$$

then the corresponding weights are obtained by

$$b_i = \int_0^1 l^{s,i}(\tau) d\tau. \quad (8.29)$$

At first, we restrict our attention to the case with constant skew-symmetric matrix S , i.e.,

$$\dot{z} = S \nabla I(z). \quad (8.30)$$

Later we will generalise to the case where S depends on z , which will lead us to partitioned Runge-Kutta methods.

Definition 8.7 (Integral Preserving Collocation Methods). *Let c_1, \dots, c_s be distinct real numbers (usually $0 \leq c_i \leq 1$) for which $b_i \neq 0$ for all i . Consider polynomial approximations $z_h(t)$ of $z(t)$ of degree s , satisfying*

$$z_h(t_n) = z_n, \quad (8.31)$$

$$\dot{z}_h(t_n + c_i h) = \int_0^1 \frac{l^{s,i}(\tau)}{b_i} S \nabla I(z_h(t_n + \tau h)) d\tau. \quad (8.32)$$

The numerical solution after one time step is then defined by $z_{n+1} = z_h(t_{n+1})$ where $t_{n+1} = t_n + h$.

Remark 8.8. *Approximating the integral with the interpolatory quadrature formula corresponding to the nodes c_1, \dots, c_s , we obtain $\dot{z}_h(t_n + c_i h) = f(z_h(t_n + c_i h))$, so that the method reduces to classical collocation methods.*

We can consider two types of integrators (c.f., Galerkin integrators of 0th and 1st kind). Either we consider the coefficients of $z_h(t)$, denoted by

$$Z_{n,i} = z_h(t_n + c_i h), \quad (8.33)$$

as basic variables, or the coefficients of $\dot{z}_h(t)$, denoted by

$$\dot{Z}_{n,i} = \dot{z}_h(t_n + c_i h). \quad (8.34)$$

In the first case, the polynomial $z_h(t)$ and the derivative of $z_h(t)$ become

$$z_h(t_n + \tau h) = \sum_{i=1}^s l^{s,i}(\tau) Z_{n,i}, \quad (8.35)$$

$$\dot{z}_h(t_n + \tau h) = \sum_{i=1}^s \dot{l}^{s,i}(\tau) Z_{n,i}. \quad (8.36)$$

In the second case, the derivative of $z_h(t)$ and the polynomial $z_h(t)$ itself become

$$\dot{z}_h(t_n + \tau h) = \sum_{i=1}^s l^{s,i}(\tau) \dot{Z}_{n,i}, \quad (8.37)$$

$$z_h(t_n + \tau h) = z_n + h \sum_{i=1}^s \int_0^\tau l^{s,i}(\tau) \dot{Z}_{n,i} d\tau. \quad (8.38)$$

Inserting (8.38) into the definition of the method (8.32), we obtain a nonlinear set of equations $\dot{Z}_n = G(\dot{Z}_n)$ for the finite-dimensional vector $\dot{Z}_n = (\dot{Z}_{n,1}, \dots, \dot{Z}_{n,s})^T$ with $G : \mathbb{R}^s \rightarrow \mathbb{R}^s$. Similarly, inserting (8.35) into (8.32), we obtain a nonlinear set of equations $Z_n = \bar{G}(Z_n)$ for $Z_n = (Z_{n,1}, \dots, Z_{n,s})^T$ and $\bar{G} : \mathbb{R}^s \rightarrow \mathbb{R}^s$. In both cases, these equations can be solved by fixed-point iteration or by Newton's method.

Example 8.9. *The simplest example of a generalised collocation method is the case of $b_1 = 1$, $c_1 = 1/2$, and approximating \dot{z} with piecewise constants, so that the polynomial z_h and its time derivative \dot{z}_h become*

$$\dot{z}_h(t)|_{[t_n, t_{n+1}]} = \dot{z}_{n+1/2}, \quad z_h(t_n + \tau h) = z_n + h \int_0^\tau \dot{z}_{n+1/2} d\tau = z_n + h\tau \dot{z}_{n+1/2}. \quad (8.39)$$

Equation (8.32) yields

$$\dot{z}_h(t_n + h/2) = \int_0^1 S \nabla I(z_n + h\tau \dot{z}_{n+1/2}) d\tau. \quad (8.40)$$

Using that

$$\dot{z}_h(t_n + h/2) = \dot{z}_{n+1/2},$$

as well as

$$z_{n+1} = z_h(t_{n+1}) = z_n + h \dot{z}_{n+1/2},$$

and thus

$$\dot{z}_{n+1/2} = \frac{z_{n+1} - z_n}{h},$$

we obtain

$$\frac{z_{n+1} - z_n}{h} = \int_0^1 S \nabla I(z_n + \tau(z_{n+1} - z_n)) d\tau, \quad (8.41)$$

which is just the average vector field method,

$$\frac{z_{n+1} - z_n}{h} = \int_0^1 S \nabla I((1 - \tau)z_n + \tau z_{n+1}) d\tau. \quad (8.42)$$

Example 8.10. Consider the reverse of the previous example, namely choosing $b_1 = b_2 = 1/2$, $c_1 = 0$, $c_2 = 1$, and approximating z with piecewise linear polynomials, leading to

$$z_h(t)|_{[t_n, t_{n+1}]} = z_n \frac{t_{n+1} - t}{h} + z_{n+1} \frac{t - t_n}{h}, \quad \dot{z}_h(t)|_{[t_n, t_{n+1}]} = \frac{z_{n+1} - z_n}{h}. \quad (8.43)$$

Using $z_h(t_n) = z_n$ and $z_h(t_{n+1}) = z_{n+1}$ we immediately identified $Z_{n,1} = z_n$ and $Z_{n,2} = z_{n+1}$. Equation (8.32) yields

$$\dot{z}_h(t_n) = 2 \int_0^1 (1 - \tau) S \nabla I((1 - \tau)z_n + \tau z_{n+1}) d\tau, \quad (8.44)$$

$$\dot{z}_h(t_n + h) = 2 \int_0^1 \tau S \nabla I((1 - \tau)z_n + \tau z_{n+1}) d\tau. \quad (8.45)$$

Using that

$$\dot{z}_h(t_n) = \dot{z}_h(t_n + h) = \frac{z_{n+1} - z_n}{h},$$

and averaging over the two expressions, we obtain

$$\frac{z_{n+1} - z_n}{h} = \int_0^1 S \nabla I((1 - \tau)z_n + \tau z_{n+1}) d\tau, \quad (8.46)$$

which is again recognised as the average vector field method.

The computation of $G(\dot{Z}_n)$ or $\bar{G}(Z_n)$ requires the computation of integrals, which can be computed exactly for polynomial vector fields or approximated numerically by accurate quadrature formula. If r is the order of the quadrature formula based on the nodes c_1, \dots, c_s , then the generalised collocation methods has

$$\text{order} = \begin{cases} 2s & \text{for } r > 2s - 2, \\ 2r - 2s + 2 & \text{for } r \leq 2s - 2. \end{cases} \quad (8.47)$$

Now we want to generalise these methods to the case of z dependent matrix S [17], that is

$$\dot{z} = S(z) \nabla I(z). \quad (8.48)$$

The simplest example of such a method is

$$\frac{z_{n+1} - z_n}{h} = S\left(\frac{z_n + z_{n+1}}{2}\right) \int_0^1 \nabla I((1 - \tau)z_n + \tau z_{n+1}) d\tau, \quad (8.49)$$

which in the case of constant S reduces to the average vector field method. For variable S , this corresponds to the average discrete gradient with a midpoint discretisation of S .

Definition 8.11 (Generalised Integral Preserving Collocation Methods). Let c_1, \dots, c_s be distinct real numbers (usually $0 \leq c_i \leq 1$) for which $b_i \neq 0$ for all i . Consider polynomial approximations $z_h(t)$ of $z(t)$ of degree s , satisfying

$$z_h(t_n) = z_n, \quad (8.50)$$

$$\dot{z}_h(t_n + c_i h) = S(z_h(t_n + c_i h)) \int_0^1 \frac{l_i(\tau)}{b_i} \nabla I(z_h(t_n + \tau h)) d\tau. \quad (8.51)$$

The numerical solution after one time step is then defined by $z_{n+1} = z_h(t_{n+1})$ where $t_{n+1} = t_n + h$.

As the factors $S(z)$ and $I(z)$ are treated differently, this method should be considered as a partitioned method.

8.4 Symplecticity and Energy Preservation

The following two theorems limit the possibility of constant time stepping algorithms to be symplectic and energy preserving at the same time. The first theorem refers to nonintegrable Hamiltonian systems, that is systems which do not admit other independent first integrals different from the Hamiltonian.

Theorem 8.12 (Zhong and Marsden [80]). *If a symplectic map φ_h conserves the Hamiltonian $H(z)$ exactly, then φ_h is identical to the exact flow of the system up to a reparametrisation of time.*

The second theorem applies to general (not necessarily non-integrable) Hamiltonian systems, but restricts to B-Series methods.

Theorem 8.13 (Chartier, Faou, and Murua [15]). *The only symplectic B-Series method that conserves the Hamiltonian $H(z)$ is the exact flow of the differential equation.*

However, it is possible to construct time-step dependent algorithms, which are symplectic and energy preserving at the same time.

8.5 Energy Preserving Symplectic Runge-Kutta Methods

One family of symplectic Runge-Kutta methods we considered are Gauss collocation methods, which are of order $2s$ with s denoting the number of stages. The Gauss collocation methods can be modified [9] by introducing a real parameter α in such a way that the resulting method remains symplectic, although the order is reduced to $2s - 2$. Under suitable assumptions, the parameter α may be tuned, at each step of the integration procedure, so as to guarantee energy conservation as well as to maintain the original order $2s$.

More precisely, consider a family of one-step methods

$$z_{n+1}(\alpha) = \varphi_h(z_n, \alpha), \quad (8.52)$$

depending on a real parameter α , with the following specifics.

1. For any fixed $\alpha \neq 0$, the corresponding method is a symplectic Runge-Kutta method with s stages and of order $2s - 2$.
2. For $\alpha = 0$ the Gauss collocation methods (of order $2s$) are recovered.
3. For any z_n and in a given range of the step size h , there exists a value of α denoted by α^* , depending on both z_n and h , such that $H(z_{n+1}) = H(z_n)$.

Under suitable assumptions, there exists a real sequence $\{\alpha_n\}_{n=0}^N$ such that the numerical solution defined by $z_{n+1} = \varphi_h(z_n, \alpha_n)$ satisfies $H(z_n) = H(z_0)$ for all n . This is not in contradiction to the above nonexistence results, as the energy conservation property only applies to the specific numerical trajectory $\{z_n\}_{n=0}^N$ obtained from the method starting with initial value z_0 and time step h . Choosing a different initial value z_0^* or a different time step h^* , the same sequence $\{\alpha_n\}_{n=0}^N$ will not assure energy conservation, but instead a different sequence $\{\alpha_n^*\}_{n=0}^N$ has to be used. This

corresponds to a weakened version of the standard energy conservation conditioned mentioned in the nonexistence theorems.

In order to define the methods, denote by $c_1 < \dots < c_s$ and b_1, \dots, b_s the nodes and weights of the Gauss-Legendre quadrature formula in the interval $[0, 1]$. Consider Legendre polynomials $P^{s,j}(\tau)$ of order s for $j = 1, \dots, s$, shifted and normalised in the interval $[0, 1]$, so that

$$\int_0^1 P^{s,i}(\tau) P^{s,j}(\tau) d\tau = \delta^{ij}, \quad 1 \leq i, j \leq s. \quad (8.53)$$

Denote by \mathcal{P} the $s \times s$ matrix

$$\mathcal{P} = \begin{pmatrix} P^{s,1}(c_1) & P^{s,2}(c_1) & \dots & P^{s,s}(c_1) \\ P^{s,1}(c_2) & P^{s,2}(c_2) & \dots & P^{s,s}(c_2) \\ \vdots & \vdots & \ddots & \vdots \\ P^{s,1}(c_s) & P^{s,2}(c_s) & \dots & P^{s,s}(c_s) \end{pmatrix}. \quad (8.54)$$

The Butcher array A of the Gauss collocation method of order $2s$ can be decomposed as [34, Chapter 19, Theorem 5.6]

$$A = \mathcal{P} X_s \mathcal{P}^{-1}, \quad (8.55)$$

with X_s defined as

$$X_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \end{pmatrix}, \quad (8.56)$$

and

$$\xi_j = \frac{1}{2\sqrt{(2j+1)(2j-1)}}, \quad 1 \leq j \leq s-1. \quad (8.57)$$

A new family of methods is obtained by perturbing X_s in the following way

$$X_s \rightarrow X_s^\alpha = X_s + \alpha W_s, \quad (8.58)$$

where α is a real parameter and

$$W_s = \begin{pmatrix} 0 & 0 & & \\ 0 & 0 & \ddots & \\ & \ddots & \ddots & -1 \\ & & 1 & 0 \end{pmatrix}, \quad (8.59)$$

so that X_s^α is a rank two perturbation of X_s . The new family of methods $z_{n+1} = \varphi_h(z_n, \alpha)$ we are interested in is defined by the following Butcher tableau,

$$\begin{array}{c|c} c_1 & \mathcal{A}(\alpha) \\ \vdots & \\ c_s & \\ \hline & b_1 \dots b_s \end{array}, \quad (8.60)$$

where

$$\mathcal{A}(\alpha) \equiv \mathcal{P} X_s^\alpha \mathcal{P}^{-1} = A + \alpha \mathcal{P} W_s \mathcal{P}^{-1}, \quad (8.61)$$

so that $\mathcal{A}(0) = A$. For $s = 2$, the tableau (8.60) becomes

$$\begin{array}{c|cc} \frac{1}{2} - \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{4} - \frac{1}{6}\sqrt{3} - \alpha \\ \frac{1}{2} + \frac{1}{6}\sqrt{3} & \frac{1}{4} + \frac{1}{6}\sqrt{3} + \alpha & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}. \quad (8.62)$$

Theorem 8.14. *For any value of α , the Runge-Kutta method defined by (8.60) is symplectic. Consequently it preserves all quadratic invariants of the continuous dynamical system.*

Proof. See [9, Theorem 2.1]. □

In the event that a value $\alpha^* \equiv \alpha^*(z_n, h)$ for the parameter α may be found such that the conservation condition $H(\varphi_h(z_{n+1}, \alpha^*)) = H(z_n)$ is satisfied, the parametric method (8.60) provides a symplectic scheme

$$z \mapsto \varphi_h(z, \alpha^*), \quad (8.63)$$

that preserves energy if evaluated at z_n . The existence of such an α^* is proved in [9, Section 3].

Theorem 8.15. *If for the family of methods (8.60) the parameter α is a function of the time step h in such a way that $\alpha(h) = \mathcal{O}(h^2)$. Then the resulting method has order $2s$.*

Proof. See [9, Theorem 3.3]. □

In [9, Theorem 3.2] it is shown that there exists a function $\alpha^*(h)$ which satisfies this criterion and is such that $H(\varphi_h(z_{n+1}, \alpha^*)) = H(z_n)$.

8.6 Energy Preserving Variational Integrators

In the framework of variational integrators, symplectic energy-momentum preserving integrators can be obtained by stressing the space-time view of classical mechanics. In addition to standard variational integrators, energy preservation is imposed, in order to compute the time steps. This leads to a slight modification of the meaning of the term symplectic in the context of adaptive time stepping algorithms, which is necessary as these algorithms are not given by a single mapping associated with a constant time step. The varying time step places us in the realms of time dependent mechanics.

8.6.1 Energy Conservation from Hamilton's Principle

Energy conservation is obtained by considering transformations of time,

$$t \mapsto \xi^\epsilon(t) = \xi(t, \epsilon) \quad \text{such that} \quad \xi^0 = \text{id} \quad \text{and} \quad \xi^\epsilon(0) = 0, \xi^\epsilon(T) = T. \quad (8.64)$$

The corresponding vector field is given by

$$X = \left. \frac{d\xi^\epsilon}{d\epsilon} \right|_{\epsilon=0}. \quad (8.65)$$

The transformation in t induces a transformation of the coordinates $q(\xi^\epsilon(t))$, whose vector field is given by

$$\bar{X}(q) = \left. \frac{d(q \circ \xi^\epsilon)}{d\epsilon} \right|_{\epsilon=0} = \left. \frac{dq}{dt} \frac{d\xi^\epsilon}{d\epsilon} \right|_{\epsilon=0}, \quad (8.66)$$

so that in components

$$\bar{X} = X v^i \frac{\partial}{\partial x^i}, \quad (8.67)$$

where by slight abuse of notation we denote the component of X also by X . Applying Hamilton's principle of stationary action for this transformation, we obtain

$$\delta \mathcal{A}[q] = d\mathcal{A}[q] \cdot \bar{X} = \int_0^T \left[\frac{\partial L}{\partial x}(q, \dot{q}) \cdot \bar{X} + \frac{\partial L}{\partial v}(q, \dot{q}) \cdot \dot{\bar{X}} \right] dt = 0. \quad (8.68)$$

Integrating the second term in square brackets by parts and using the particular form of the variations, this becomes

$$\begin{aligned} d\mathcal{A}[q] \cdot \bar{X} &= \int_0^T \left[\frac{\partial L}{\partial x}(q, \dot{q}) - \frac{d}{dt} \left(\frac{\partial L}{\partial v}(q, \dot{q}) \right) \right] \cdot \bar{X} dt \\ &= \int_0^T \left[\frac{\partial L}{\partial x}(q, \dot{q}) - \frac{d}{dt} \left(\frac{\partial L}{\partial v}(q, \dot{q}) \right) \right] \cdot \dot{q} X dt = 0. \end{aligned} \quad (8.69)$$

As X is arbitrary, this implies

$$\frac{dE}{dt} = \left[\frac{\partial L}{\partial x}(q, \dot{q}) - \frac{d}{dt} \left(\frac{\partial L}{\partial v}(q, \dot{q}) \right) \right] \cdot \dot{q} = 0, \quad (8.70)$$

where

$$E = \frac{\partial L}{\partial v}(q, \dot{q}) \cdot \dot{q} - L(q, \dot{q}). \quad (8.71)$$

This shows how the Hamiltonian arises naturally when considering variations of the curve $q(t)$ that originate from time reparametrisations.

8.6.2 Discrete Action Principle

This suggests that in order to obtain an energy conserving variational integrator, we must allow for such reparametrisations of time on the discrete level. This is accomplished by using a variable time step $h_{n,n+1} = t_{n+1} - t_n$ instead of a constant h for all integration steps. This implies the discrete Lagrangian L_d becomes a functions not only of q_n and q_{n+1} but also of t_n and t_{n+1} . The trapezoidal and midpoint approximations of the exact discrete Lagrangians, introduced before for constant time steps h , therefore become

$$L_d^{\text{tr}}(q_n, q_{n+1}, t_n, t_{n+1}) = \frac{t_{n+1} - t_n}{2} \left[L\left(q_n, \frac{q_{n+1} - q_n}{t_{n+1} - t_n}\right) + L\left(q_{n+1}, \frac{q_{n+1} - q_n}{t_{n+1} - t_n}\right) \right], \quad (8.72)$$

and

$$L_d^{\text{mp}}(q_n, q_{n+1}, t_n, t_{n+1}) = (t_{n+1} - t_n) L\left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{t_{n+1} - t_n}\right), \quad (8.73)$$

respectively. Requiring stationarity of the corresponding discrete action (Hamilton's principle),

$$\delta \mathcal{A}_d[q_d, t_d] = \delta \sum_{n=0}^{N-1} L_d(q_n, q_{n+1}, t_n, t_{n+1}) = 0, \quad (8.74)$$

where $t_d = \{t_n\}_{n=0}^N$, we obtain the extended discrete Euler-Lagrange equations, namely

$$D_1 L_d(q_n, q_{n+1}, t_n, t_{n+1}) + D_2 L_d(q_{n-1}, q_n, t_{n-1}, t_n) = 0, \quad (8.75a)$$

$$D_3 L_d(q_n, q_{n+1}, t_n, t_{n+1}) + D_4 L_d(q_{n-1}, q_n, t_{n-1}, t_n) = 0. \quad (8.75b)$$

The first equation originates from variations in the discrete trajectories q_d while the second equation originates from variations in the time points t_d . The Euler-Lagrange equations for q are coupled with an energy equation that enables us to solve for both q_{n+1} and t_{n+1} at the same time.

8.6.3 Discrete Energy Conservation

Similar to the discrete momenta, we define the discrete energies

$$E_{L_d}^+(q_n, q_{n+1}, t_n, t_{n+1}) = -D_4 L_d(q_n, q_{n+1}, t_n, t_{n+1}), \quad (8.76a)$$

$$E_{L_d}^-(q_n, q_{n+1}, t_n, t_{n+1}) = D_3 L_d(q_n, q_{n+1}, t_n, t_{n+1}), \quad (8.76b)$$

so that the second component of the discrete Euler-Lagrange equations read

$$E_{L_d}^+(q_{n-1}, q_n, t_{n-1}, t_n) = E_{L_d}^-(q_n, q_{n+1}, t_n, t_{n+1}). \quad (8.77)$$

which reflects the evolution of the discrete energy. If the discrete Lagrangian is invariant with respect to transformations in time of the form $t \mapsto t + \epsilon\tau$, that is

$$L_d(q_n, q_{n+1}, t_n + \epsilon\tau, t_{n+1} + \epsilon\tau) = L_d(q_n, q_{n+1}, t_n, t_{n+1}), \quad (8.78)$$

then taking derivatives with respect to ϵ shows that

$$\begin{aligned} & \left. \frac{d}{d\epsilon} L_d(q_n, q_{n+1}, t_n + \epsilon\tau, t_{n+1} + \epsilon\tau) \right|_{\epsilon=0} \\ &= \left[D_3 L_d(q_n, q_{n+1}, t_n, t_{n+1}) + D_4 L_d(q_n, q_{n+1}, t_n, t_{n+1}) \right] \tau = 0 \quad \text{for all } \tau, \end{aligned} \quad (8.79)$$

and thus

$$E_{L_d}^+(q_n, q_{n+1}, t_n, t_{n+1}) = E_{L_d}^-(q_n, q_{n+1}, t_n, t_{n+1}). \quad (8.80)$$

Combining this with the time-component of the Euler-Lagrange equations yields

$$E_{L_d}^+(q_{n-1}, q_n, t_{n-1}, t_n) = E_{L_d}^+(q_n, q_{n+1}, t_n, t_{n+1}), \quad (8.81a)$$

$$E_{L_d}^-(q_{n-1}, q_n, t_{n-1}, t_n) = E_{L_d}^-(q_n, q_{n+1}, t_n, t_{n+1}), \quad (8.81b)$$

which shows that time invariant of the discrete Lagrangian leads to conservation of the discrete energies.

Example 8.16. *In the particular case of the midpoint Lagrangian, the discrete energies take the form*

$$\begin{aligned}
 E_{L_d}^+(q_n, q_{n+1}, t_n, t_{n+1}) &= -D_4 L_d(q_n, q_{n+1}, t_n, t_{n+1}) \\
 &= \frac{q_{n+1} - q_n}{t_{n+1} - t_n} \frac{\partial L}{\partial v} \left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{t_{n+1} - t_n} \right) - L \left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{t_{n+1} - t_n} \right), \\
 E_{L_d}^-(q_n, q_{n+1}, t_n, t_{n+1}) &= D_3 L_d(q_n, q_{n+1}, t_n, t_{n+1}) \\
 &= \frac{q_{n+1} - q_n}{t_{n+1} - t_n} \frac{\partial L}{\partial v} \left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{t_{n+1} - t_n} \right) - L \left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{t_{n+1} - t_n} \right),
 \end{aligned}$$

which are clearly an approximation of the continuous energy. Both expressions are immediately seen to be identical, which is expected as the continuous Lagrangian does not have an explicit time dependence.

9 Constraints and Forces

Lagrangian and Hamiltonian systems subject to constraints and external forcing arise in many applications. When integrating such systems numerically, it is important to do so in a structure-preserving way in order to avoid spurious numerical artefacts.

We will first discuss forced systems and how to discretise them. To large extend, the discretisation of constraint systems then follows in an analogous way as the action of the constraints can be seen as exerting forces on the unconstrained system.

We will consider various classes of constraints, holonomic, nonholonomic and in the next chapter also Dirac constraints. Holonomic constraints are easiest to deal with as they are variational and can be incorporated into the action principle via Lagrange multipliers. Nonholonomic constraints are more subtle as they are not variational. For their treatment it is necessary to modify Hamilton's action principle, leading to the Lagrange-d'Alembert principle.

9.1 Forced Systems

In the following, we will discuss how to incorporate external, non-potential forces into the Lagrangian and Hamiltonian framework of classical mechanics and how to account for such forces in numerical integration methods.

9.1.1 Forced Lagrangian Systems

Recall that a Lagrangian system is characterised by three objects, the configuration space \mathcal{M} , the Lagrangian $L : T\mathcal{M} \rightarrow \mathbb{R}$ and the Euler-Lagrange equations,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \mathbf{v}}(q(t), \dot{q}(t)) \right) - \frac{\partial L}{\partial \mathbf{x}}(q(t), \dot{q}(t)) = 0, \quad (9.1)$$

which are equivalent to Hamilton's principle of stationary action,

$$\delta \int_{t_1}^{t_2} L(q(t), \dot{q}(t)) dt = 0, \quad (9.2)$$

with $q(t)$ taking fixed values at t_1 and t_2 so that $\delta q(t_1) = \delta q(t_2) = 0$. In the presence of external forces F_L , such as friction, Hamilton's principle is modified to the Lagrange-d'Alembert principle,

$$\delta \int_{t_1}^{t_2} L(q(t), \dot{q}(t)) dt + \int_{t_1}^{t_2} F_L(q(t), \dot{q}(t)) \cdot \delta q dt = 0, \quad (9.3)$$

which is equivalent to the Euler-Lagrange equations with external forces,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \mathbf{v}}(q(t), \dot{q}(t)) \right) - \frac{\partial L}{\partial \mathbf{x}}(q(t), \dot{q}(t)) = F_L(q(t), \dot{q}(t)). \quad (9.4)$$

9.1.2 Fibre Derivative with Forces

The Lagrangian forces F_L can be related to their Hamiltonian counterparts F_H with the help of the standard fibre derivative $\mathbb{F}L : \mathcal{T}\mathcal{M} \rightarrow \mathcal{T}^*\mathcal{M}$ by

$$F_L = F_H \circ \mathbb{F}L. \quad (9.5)$$

If the Lagrangian L is regular, so that we can define a corresponding Hamiltonian H by the Legendre transform, it can be shown that the forced Lagrangian vector field X_L is equivalent to the forced Hamiltonian vector field X_H by

$$X_L = (\mathbb{F}L)^* X_H, \quad (9.6)$$

and the forced Euler-Lagrange equations are equivalent to the forced Hamilton equations.

9.1.3 Forced Hamiltonian Systems

In local coordinates, the forced Hamiltonian vector field is given by

$$X_H = X_{x^i} \frac{\partial}{\partial x^i} + X_{p_i} \frac{\partial}{\partial p^i}, \quad (9.7)$$

with

$$X_x = \frac{\partial H}{\partial x}(q(t), p(t)), \quad X_p = -\frac{\partial H}{\partial p}(q(t), p(t)) + F_H(q(t), p(t)), \quad (9.8)$$

so that the Hamilton equations,

$$\frac{d}{dt} z(t) = X_H(z(t)), \quad (9.9)$$

become

$$\dot{q}(t) = \frac{\partial H}{\partial p}(q(t), p(t)), \quad \dot{p}(t) = -\frac{\partial H}{\partial x}(q(t), p(t)) + F_H(q(t), p(t)), \quad (9.10)$$

which can be shown to be equivalent to the forced Euler-Lagrange equations.

9.1.4 Noether Theorem with Forces

If the ideal system, without external forces, has variational symmetries and therefore obeys some conservation laws, these conservation laws will, in general, be altered in the presence of the forces. However, in the special case of the forces being orthogonal to the symmetry generators, the conservation laws stay intact.

Considering an infinitesimal transformation

$$q(t) \rightarrow q^\epsilon(t) = \sigma(t, q(t), \epsilon) = \sigma^\epsilon(t, q(t)) \quad \text{with} \quad \sigma^0 = \text{id}, \quad \text{and} \quad X = \left. \frac{d\sigma^\epsilon}{d\epsilon} \right|_{\epsilon=0}, \quad (9.11)$$

the invariance condition on reads

$$\int_{t_1}^{t_2} \left[\frac{\partial L}{\partial x}(q, \dot{q}) \cdot X + \frac{\partial L}{\partial v}(q, \dot{q}) \cdot \dot{X} \right] dt + \int_{t_1}^{t_2} F_L(q(t), \dot{q}(t)) \cdot X dt = \int_{t_1}^{t_2} F_L(q(t), \dot{q}(t)) \cdot X dt, \quad (9.12)$$

assuming that the Lagrangian L is invariant under the transformation. Using the Euler-Lagrange equations (9.4) to replace $\partial L/\partial \dot{x}$ in (9.12), we obtain

$$\int_{t_1}^{t_2} \left[\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{v}}(q(t), \dot{q}(t)) \right) + \frac{\partial L}{\partial v}(q, \dot{q}) \cdot \dot{X} \right] dt = \int_{t_1}^{t_2} F_L(q(t), \dot{q}(t)) \cdot X dt, \quad (9.13)$$

where on the left-hand side we have a total time derivative, so that upon integration,

$$\frac{\partial L}{\partial v}(q(t_2), \dot{q}(t_2)) \cdot X(q(t_2)) - \frac{\partial L}{\partial v}(q(t_1), \dot{q}(t_1)) \cdot X(q(t_1)) = \int_{t_1}^{t_2} F_L(q(t), \dot{q}(t)) \cdot X(q(t)) dt. \quad (9.14)$$

This equation shows the evolution of the momentum from time t_1 to time t_2 , and we see that external forces will generally modify the momentum. If, however, the force happens to be orthogonal to the symmetry group action, Noether's theorem will still hold and the momentum will be preserved.

9.1.5 Discrete Lagrange–d'Alembert Principle

Similar to the discrete fibre derivative, we consider two discrete Lagrangian forces,

$$F_d^+, F_d^- : \mathcal{M} \times \mathcal{M} \rightarrow T^*\mathcal{M}, \quad (9.15)$$

which have coordinate expressions

$$F_d^+(q_n, q_{n+1}) = (q_{n+1}, F_d^+(q_n, q_{n+1})), \quad (9.16a)$$

$$F_d^-(q_n, q_{n+1}) = (q_n, F_d^-(q_n, q_{n+1})). \quad (9.16b)$$

The two discrete forces are combined to give a single one-form

$$F_d : \mathcal{M} \times \mathcal{M} \rightarrow T^*(\mathcal{M} \times \mathcal{M}), \quad (9.17)$$

defined by

$$F_d(q_n, q_{n+1}) \cdot (\delta q_n, \delta q_{n+1}) = F_d^+(q_n, q_{n+1}) \cdot \delta q_{n+1} + F_d^-(q_n, q_{n+1}) \cdot \delta q_n. \quad (9.18)$$

With that, we can write the discrete Lagrange-d'Alembert principle,

$$\delta \sum_{n=0}^{N-1} L_n(q_n, q_{n+1}) + \sum_{n=0}^{N-1} \left[F_d^-(q_n, q_{n+1}) \cdot \delta q_n + F_d^+(q_n, q_{n+1}) \cdot \delta q_{n+1} \right] = 0, \quad (9.19)$$

seeking discrete trajectory $q_d = \{q_n\}_{n=0}^N$ for all variations $\delta q_d = \{\delta q_n\}_{n=0}^N$ vanishing at the endpoints, $\delta q_0 = \delta q_N = 0$. This is equivalent to the forced discrete Euler-Lagrange equations,

$$D_1 L_d(q_n, q_{n+1}) + D_2 L_d(q_{n-1}, q_n) + F_d^-(q_n, q_{n+1}) + F_d^+(q_{n-1}, q_n) = 0, \quad (9.20)$$

which are the same as the standard discrete Euler-Lagrange equations with the discrete forces added.

9.1.6 Discrete Fibre Derivative with Forces

The forced discrete fibre derivatives are defined as

$$\mathbb{F}^{F^-} L_d : (q_n, q_{n+1}) \mapsto (q_n, p_n) = (q_n, -D_1 L_d(q_n, q_{n+1}) - F_d^-(q_n, q_{n+1})), \quad (9.21a)$$

$$\mathbb{F}^{F^+} L_d : (q_n, q_{n+1}) \mapsto (q_{n+1}, p_{n+1}) = (q_{n+1}, D_2 L_d(q_n, q_{n+1}) + F_d^+(q_n, q_{n+1})). \quad (9.21b)$$

With this, the position-momentum form of the forced variational integrator is given by

$$p_n = -D_1 L_d(q_n, q_{n+1}) - F_d^-(q_n, q_{n+1}), \quad (9.22a)$$

$$p_{n+1} = D_2 L_d(q_n, q_{n+1}) + F_d^+(q_n, q_{n+1}), \quad (9.22b)$$

which is the same as the standard position-momentum form with the discrete forces added.

9.1.7 Discrete Noether Theorem with Forces

Consider a one parameter group of discrete curves $q_d^\epsilon = \{q_n^\epsilon\}_{n=0}^N$ with

$$q_n^\epsilon = \sigma^\epsilon(t_n, q_n), \quad \text{with} \quad \sigma^0 = \text{id}, \quad \text{and} \quad X_{\mathcal{M}} = \left. \frac{\partial \sigma^\epsilon}{\partial \epsilon} \right|_{\epsilon=0}, \quad (9.23)$$

where σ^ϵ is the same function as in the continuous case. The generating vector field $X_{\mathcal{M}}$ is lifted from \mathcal{M} to the product $\mathcal{M} \times \mathcal{M}$ by

$$X_{\mathcal{M} \times \mathcal{M}}(q_n, q_{n+1}) = X_{\mathcal{M}}(q_n) \frac{\partial}{\partial x_n} + X_{\mathcal{M}}(q_{n+1}) \frac{\partial}{\partial x_{n+1}}. \quad (9.24)$$

Then the invariance condition reads

$$\begin{aligned} \sum_{n=0}^{N-1} dL_d(q_n, q_{n+1}) \cdot X_{\mathcal{M} \times \mathcal{M}}(q_n, q_{n+1}) + \sum_{n=0}^{N-1} F_d(q_n, q_{n+1}) \cdot X_{\mathcal{M} \times \mathcal{M}}(q_n, q_{n+1}) = \\ = \sum_{n=0}^{N-1} F_d(q_n, q_{n+1}) \cdot X_{\mathcal{M} \times \mathcal{M}}(q_n, q_{n+1}), \end{aligned} \quad (9.25)$$

where

$$dL_d(q_n, q_{n+1}) \cdot X_{\mathcal{M} \times \mathcal{M}}(q_n, q_{n+1}) = D_1 L_d(q_n, q_{n+1}) \cdot X_{\mathcal{M}}(q_n) + D_2 L_d(q_n, q_{n+1}) \cdot X_{\mathcal{M}}(q_{n+1}). \quad (9.26)$$

and

$$F_d(q_n, q_{n+1}) \cdot X_{\mathcal{M} \times \mathcal{M}}(q_n, q_{n+1}) = F_d^-(q_n, q_{n+1}) \cdot X_{\mathcal{M}}(q_n) + F_d^+(q_n, q_{n+1}) \cdot X_{\mathcal{M}}(q_{n+1}). \quad (9.27)$$

From the invariance condition (9.25) we obtain the expression

$$\begin{aligned} \sum_{n=1}^{N-1} \left[D_1 L_d(q_n, q_{n+1}) + D_2 L_d(q_{n-1}, q_n) + F_d^-(q_n, q_{n+1}) + F_d^+(q_{n-1}, q_n) \right] \cdot X_{\mathcal{M}}(q_n) \\ + \left[D_1 L_d(q_0, q_1) + F_d^-(q_0, q_1) \right] \cdot X_{\mathcal{M}}(q_0) + \left[D_2 L_d(q_{N-1}, q_N) + F_d^+(q_{N-1}, q_N) \right] \cdot X_{\mathcal{M}}(q_N) \\ = \sum_{n=0}^{N-1} F_d(q_n, q_{n+1}) \cdot X_{\mathcal{M} \times \mathcal{M}}(q_n, q_{n+1}). \end{aligned} \quad (9.28)$$

Using the forced discrete Euler-Lagrange equations (9.20), the sum vanishes and the remaining terms can be rewritten with (9.22) as

$$p_N \cdot X_{\mathcal{M}}(q_N) - p_0 \cdot X_{\mathcal{M}}(q_0) = \sum_{n=0}^{N-1} F_d(q_n, q_{n+1}) \cdot X_{\mathcal{M} \times \mathcal{M}}(q_n, q_{n+1}), \quad (9.29)$$

which describes the evolution of the discrete momentum. Just as in the continuous case, if the forces are orthogonal to the symmetry generators, the right-hand side vanishes and the two momenta are equal.

9.1.8 Exact Discrete Forcing

The discrete Lagrangian should approximate the continuous action over one time step. When forces are added, this must be modified so that the discrete Lagrange-d'Alembert principle (9.19) approximates the continuous expression (9.3).

Definition 9.1. *Given a Lagrangian $L : \mathbb{T}\mathcal{M} \rightarrow \mathbb{R}$ and a Lagrangian force $F_L : \mathbb{T}\mathcal{M} \rightarrow \mathbb{T}^*\mathcal{M}$, the exact forced discrete Lagrangian $L_d^e : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R}$ and the exact discrete forces $F_d^{e-}, F_d^{e+} : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{T}^*\mathcal{M}$ are defined as*

$$L_d^e(q_n, q_{n+1}) = \int_{t_n}^{t_{n+1}} L(q_{n,n+1}(t), \dot{q}_{n,n+1}(t)) dt, \quad (9.30a)$$

$$F_d^{e-}(q_n, q_{n+1}) = \int_{t_n}^{t_{n+1}} F_L(q_{n,n+1}(t), \dot{q}_{n,n+1}(t)) \cdot \frac{\partial q_{n,n+1}(t)}{\partial q_n} dt, \quad (9.30b)$$

$$F_d^{e+}(q_n, q_{n+1}) = \int_{t_n}^{t_{n+1}} F_L(q_{n,n+1}(t), \dot{q}_{n,n+1}(t)) \cdot \frac{\partial q_{n,n+1}(t)}{\partial q_{n+1}} dt, \quad (9.30c)$$

where $q_{n,n+1}(t)$ denotes the solution of the continuous forced Euler-Lagrange equations for L and F_L in the interval $[t_n, t_{n+1}]$ satisfying the boundary conditions $q_{n,n+1}(t_n) = q_n$ and $q_{n,n+1}(t_{n+1}) = q_{n+1}$.

Remark 9.2. *Note that this exact discrete Lagrangian is not the same as that for the unforced system with Lagrangian L as the curves $q_{n,n+1}(t)$ are different.*

9.1.9 Integration of Forced Systems

In order to simulate a given forced Lagrangian system, we approximate the exact discrete Lagrangian and the exact discrete forces and consider the resulting discrete system as an integrator for the continuous problem.

Consider the discrete Lagrangian

$$L_d^\alpha(q_n, q_{n+1}) = h L\left((1-\alpha)q_n + \alpha q_{n+1}, \frac{q_{n+1} - q_n}{h}\right), \quad (9.31a)$$

for some parameter $\alpha \in [0, 1]$. For $\alpha = 1/2$, this just corresponds to the midpoint Lagrangian. The natural discrete forces for this Lagrangian are

$$F_d^{\alpha-}(q_n, q_{n+1}) = (1-\alpha)h F_L\left((1-\alpha)q_n + \alpha q_{n+1}, \frac{q_{n+1} - q_n}{h}\right), \quad (9.31b)$$

$$F_d^{\alpha+}(q_n, q_{n+1}) = \alpha h F_L\left((1-\alpha)q_n + \alpha q_{n+1}, \frac{q_{n+1} - q_n}{h}\right). \quad (9.31c)$$

In a similar way, variational partitioned Runge-Kutta methods for forced systems can be obtained. Recall that in that case the discrete Lagrangian is given by

$$L_d(q_n, q_{n+1}) = h \sum_{i=1}^s b_i L(Q_{n,i}, \dot{Q}_{n,i}). \quad (9.32a)$$

Reasonable choices of the discrete forces are

$$F_d^-(q_n, q_{n+1}) = h \sum_{i=1}^s b_i F_L(Q_{n,i}, \dot{Q}_{n,i}) \cdot \frac{\partial Q_{n,i}}{\partial q_n}, \quad (9.32b)$$

$$F_d^+(q_n, q_{n+1}) = h \sum_{i=1}^s b_i F_L(Q_{n,i}, \dot{Q}_{n,i}) \cdot \frac{\partial Q_{n,i}}{\partial q_{n+1}}, \quad (9.32c)$$

which approximate the exact discrete forces in the same way that L_d approximates the exact discrete Lagrangian.

9.2 Constrained Systems

Constrained systems appear in a larger number of difference circumstances, for example in electrical engineering or control theory. Sometimes it can also be convenient to embed a system whose dynamics takes place on a complicated manifold into a larger space and restrict the dynamics to the submanifold of interest by imposing a constraint. The corresponding dynamical equations are differential-algebraic equations, depending on both dynamical and algebraic variables.

In the following, we will first review the geometric setting of such systems, before we discuss the Lagrange multiplier theorem which is of essential importance for understanding of the treatment of constraints with the Lagrange-d'Alembert Principle. Then, in the next sections, we will review several methods for the numerical integration of systems with holonomic and nonholonomic constraints. We will always assume that the Lagrangian is hyper-regular, so that we can define a corresponding Hamiltonian.

9.2.1 Constraint Submanifolds

Consider a system defined on the manifold \mathcal{M} with coordinates $x = (x^1, \dots, x^d)$ subject to the constraint $g: \mathcal{M} \rightarrow \mathbb{R}^m$ given by

$$\begin{aligned} g^1(x^1, \dots, x^d) &= 0, \\ &\vdots \\ g^m(x^1, \dots, x^d) &= 0, \end{aligned} \quad (9.33)$$

is a system of smooth functions of rank m . The constraint $g(x) = 0$ defines a $d - m$ dimensional submanifold \mathcal{N} of \mathcal{M} , given by

$$\mathcal{N} = \{x \mid x \in \mathcal{M}, g(x) = 0\} \subset \mathcal{M}, \quad (9.34)$$

and referred to as the constraint submanifold. Note that 0 has to be a regular point of g , in order for \mathcal{N} to truly be a submanifold of \mathcal{M} . The tangent space $T_x \mathcal{N}$ at a point $x \in \mathcal{N}$ is given by

$$T_x \mathcal{N} = \{v \mid G(x)v = 0\}, \quad (9.35)$$

with $G = Dg$ the Jacobian matrix of g . Often, $G(x)v = 0$ is referred to as the hidden or secondary constraint. Correspondingly $g(x) = 0$ is often called the primary constraint. In other words, the tangent space $T_x\mathcal{N}$ can be defined as the kernel of $Dg(x)$,

$$T_x\mathcal{N} = \ker Dg(x). \quad (9.36)$$

With that, the tangent bundle of \mathcal{N} can be written as

$$T\mathcal{N} = \{(x, v) \mid x \in \mathcal{N}, v \in T_x\mathcal{N}\}, \quad (9.37)$$

or

$$T\mathcal{N} = \{(x, v) \mid x \in \mathcal{N}, v \in \ker Dg(x)\}. \quad (9.38)$$

In both cases, we have that

$$T\mathcal{N} = \{(x, v) \mid x \in \mathcal{M}, g(x) = 0, G(x)v = 0\}. \quad (9.39)$$

The cotangent space $T_x^*\mathcal{N}$ at a point $x \in \mathcal{N}$ is given by

$$T_x^*\mathcal{N} = \{p \mid G(x)H_p(x, p) = 0\}, \quad (9.40)$$

which depends not only on the derivative G of the constraint function g but also on the Hamiltonian H . With that, the cotangent bundle of \mathcal{N} can be written as

$$T^*\mathcal{N} = \{(x, p) \mid x \in \mathcal{N}, p \in T_x^*\mathcal{N}\} = \{(x, p) \mid x \in \mathcal{M}, g(x) = 0, G(x)H_p(x, p) = 0\}. \quad (9.41)$$

9.2.2 Constrained Extremisation and Lagrange Multipliers

A characterisation of extrema in terms of derivatives states that the derivatives vanish at an extremum, that is if x_0 is an extremum of the function f then $Df(x_0) = 0$. But what happens if instead of a function defined on \mathcal{M} we consider its restriction to some constraint submanifold \mathcal{N} ? It cannot be asserted that an extremum of the restricted function is a point at which the derivative of the function vanishes. The derivative of the function may vanish at points outside of \mathcal{N} . And very seldom will the derivative of the function vanish at a critical point of the restricted function. So very seldom will a constrained extremum be an unconstrained extremum and vice versa. What can be said, though, is that at an extremum x_0 of the function restricted to \mathcal{N} , the derivative of the function vanishes on all tangent vectors to \mathcal{N} at x_0 , i.e., all elements of the tangent space $T_{x_0}\mathcal{N}$.

Theorem 9.3. *Let \mathcal{N} be a submanifold of \mathcal{M} and $f : \mathcal{M} \rightarrow \mathbb{R}$ a smooth function. Denote the restriction of the function f to \mathcal{N} by $f|_{\mathcal{N}}$. A necessary condition for a point $x_0 \in \mathcal{N}$ that is non-critical for f to be a local extremum of $f|_{\mathcal{N}}$ is that*

$$T_{x_0}\mathcal{N} \subset \ker Df(x_0). \quad (9.42)$$

Proof. Choose an arbitrary vector $v \in T_{x_0}\mathcal{N}$ and a smooth path $q = q(t)$ on \mathcal{N} that passes through x_0 at $t = 0$, so that $q(0) = x_0$, and for which the vector v is the velocity at $t = 0$, that is

$$\frac{dq}{dt}(0) = v. \quad (9.43)$$

If x_0 is an extremum of $f|_{\mathcal{N}}$, the smooth function $t \mapsto f(q(t))$ must have an extremum at $t = 0$. By the necessary condition for an extremum, its derivative must vanish at $t = 0$, that is

$$\left. \frac{d}{dt} f(q(t)) \right|_{t=0} = DF(q(0)) \cdot \frac{dq}{dt}(0), \quad (9.44)$$

and so we must have

$$Df(x_0) \cdot v = 0, \quad (9.45)$$

where

$$Df(x_0) = \left(\frac{\partial f}{\partial x^1}, \dots, \frac{\partial f}{\partial x^d} \right), \quad v = (v^1, \dots, v^d). \quad (9.46)$$

Assuming that x_0 is a non-critical point of f , this condition is equivalent to $v \in \ker Df(x_0)$. \square

If \mathcal{N} is characterised by a constraint $g(x) = 0$, then as $T_x \mathcal{N} = \ker Dg(x)$ this implies that $x_0 \in \mathcal{N}$ is a local extremum of f restricted to \mathcal{N} if

$$\ker Dg(x_0) \subset \ker Df(x_0). \quad (9.47)$$

This leads us to the Lagrange multiplier theorem.

Theorem 9.4 (Lagrange Multiplier Theorem). *Let $\mathcal{N} \subset \mathcal{M}$ be a manifold known by a vector-valued function g . If a smooth function $f : \mathcal{M} \rightarrow \mathbb{R}$ restricted to \mathcal{N} has a critical point at $x \in \mathcal{N}$, then there exist numbers $\lambda_1, \dots, \lambda_m$ such that the derivative of f at x is a linear combination of the derivatives of the constraint functions,*

$$\text{grad } f(x) = \lambda_1 \text{grad } g_1(x) + \dots + \lambda_m \text{grad } g_m(x). \quad (9.48)$$

The numbers $\lambda_1, \dots, \lambda_m$ are called Lagrange multipliers.

This follows from the following lemma from linear algebra, setting $\alpha_i = \text{grad } g_i(x)$ and $\beta = \text{grad } f(x)$.

Lemma 9.5. *Let $A : \mathbb{R}^n \rightarrow \mathbb{R}^m$ be a linear transformation (that is a $m \times n$ matrix), given by*

$$A = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_m \end{bmatrix}, \quad (9.49)$$

and $\beta : \mathbb{R}^n \rightarrow \mathbb{R}$ a linear function (that is a row matrix n wide). Then

$$\ker A \subset \ker \beta \quad (9.50)$$

if and only if there exist numbers $\lambda_1, \dots, \lambda_m$ such that

$$\beta = \lambda_1 \alpha_1 + \dots + \lambda_m \alpha_m. \quad (9.51)$$

Lagrange proposed using an auxiliary function \bar{f} for seeking a constrained extremum,

$$\bar{f}(x, \lambda) = f(x) - \lambda^T g(x), \quad (9.52)$$

depending on $d+m$ variables $(x, \lambda) = (x^1, \dots, x^d, \lambda^1, \dots, \lambda^m)$. This function is convenient because the necessary conditions for an extremum of it are precisely (9.48) and (9.33), as

$$\frac{\partial \bar{f}}{\partial x^j}(q, \lambda) = \frac{\partial f}{\partial x^j}(q) - \sum_{i=1}^m \lambda^i \frac{\partial g^i}{\partial x^j}(q) = 0, \quad (j = 1, \dots, d), \quad (9.53)$$

$$\frac{\partial \bar{f}}{\partial \lambda^i}(q, \lambda) = -g^i(x) = 0, \quad (i = 1, \dots, m). \quad (9.54)$$

Thus, in seeking an extremum of a function f whose variables are subject to the constraints (9.33), one can write the function (9.52) with undetermined multipliers and look for its critical points. In other words, the following are equivalent:

(a) $x_0 \in \mathcal{N}$ is an extremum of $f|_{\mathcal{N}}$,

(a) $(q, \lambda) \in \mathcal{M} \times \mathbb{R}^m$ is an extremum of \bar{f} .

The multipliers λ are uniquely determined if the vectors $\text{grad } g^i(x_0)$ are linearly independent. This is equivalent to the statement that the rank of the system (9.33) is m .

9.3 Holonomic Constraints

Holonomic constraints are constraints on the configuration manifold of a system, that is we have a constraint function $g : \mathcal{M} \rightarrow \mathbb{R}^m$ and the constraint submanifold is given by $\mathcal{N} = g^{-1}(0) \subset \mathcal{M}$. If $i : \mathcal{N} \rightarrow \mathcal{M}$ is the embedding map,

$$i(\mathcal{N}) = \{x \in \mathcal{M} \mid g(x) = 0\}, \quad (9.55)$$

then $Ti : T\mathcal{N} \rightarrow T\mathcal{M}$, given by

$$Ti(T\mathcal{N}) = \{(x, v) \in T\mathcal{M} \mid g(x) = 0, G(x)v = 0\}, \quad (9.56)$$

provides a canonical way to embed $T\mathcal{N}$ in $T\mathcal{M}$ and we will thus regard $T\mathcal{N}$ as a submanifold of $T\mathcal{M}$. This is useful, as it allows us to restrict L to \mathcal{N} which we denote by $L|_{T\mathcal{N}}$. The corresponding action is denoted by $\mathcal{A}|_{\mathcal{N}}$.

Consider curves $q(t)$ on the time interval $[t_1, t_2] \in \mathbb{R}$ with fixed endpoints $q_1, q_2 \in \mathcal{N} \subset \mathcal{M}$. Denote by $\mathcal{Q}(\mathcal{M})$ the same of smooth functions $q : [t_1, t_2] \rightarrow \mathcal{M}$ satisfying $q(t_1) = q_1$ and $q(t_2) = q_2$, that is

$$\mathcal{Q}(\mathcal{M}) = \{q : [t_1, t_2] \rightarrow \mathcal{M} \mid q(t_1) = q_1, q(t_2) = q_2\}, \quad (9.57)$$

and correspondingly

$$\mathcal{Q}(\mathcal{N}) = \{q : [t_1, t_2] \rightarrow \mathcal{N} \mid q(t_1) = q_1, q(t_2) = q_2\}. \quad (9.58)$$

Further, denote by $\mathcal{Q}(\mathbb{R}^m)$ the space of curves $\lambda : [t_1, t_2] \rightarrow \mathbb{R}^m$ with no boundary conditions, and more generally by $\mathcal{Q}(P)$ the space of curves $[t_1, t_2] \rightarrow P$ with appropriate boundary conditions.

Theorem 9.6. *Given a Lagrangian system $L : T\mathcal{M} \rightarrow \mathbb{R}$ with holonomic constraint $g : \mathcal{M} \rightarrow \mathbb{R}^m$, set $\mathcal{N} = g^{-1}(0) \subset \mathcal{M}$ and $L|_{T\mathcal{N}}$ the restriction of L to $T\mathcal{N}$. Then the following are equivalent:*

(a) $q \in \mathcal{Q}(\mathcal{M})$ and $\lambda \in \mathcal{Q}(\mathbb{R}^m)$ satisfy the constrained Euler-Lagrange equations

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{v}}(q(t), \dot{q}(t)) \right) - \frac{\partial L}{\partial x}(q(t), \dot{q}(t)) = \langle \lambda(t), \nabla g(q(t)) \rangle, \quad (9.59a)$$

$$0 = g(q(t)), \quad (9.59b)$$

(b) $(q, \lambda) \in \mathcal{Q}(\mathcal{M} \times \mathbb{R}^m)$ extremises

$$\bar{\mathcal{A}}[q, \lambda] = \mathcal{A}[q] - \int \langle \lambda, g(q) \rangle dt, \quad (9.60)$$

and hence solves the Euler-Lagrange equations for the augmented Lagrangian $\bar{L} : T(\mathcal{M} \times \mathbb{R}^m) \rightarrow \mathbb{R}$, defined by

$$\bar{L}(q, \lambda, \dot{q}, \dot{\lambda}) = L(q, \dot{q}) - \langle \lambda, g(q) \rangle, \quad (9.61)$$

(c) $q \in \mathcal{Q}(\mathcal{N})$ extremises $\mathcal{A}|_{\mathcal{N}}$ and hence solves the Euler-Lagrange equations for $L|_{T\mathcal{N}}$.

Proof. See exercises. □

The term on the right-hand side of the constrained Euler-Lagrange equations (9.59a) has the form of a force,

$$F = \lambda^T \nabla g(q), \quad g(q) = 0, \quad (9.62)$$

acting on the Lagrangian system. This force is called the constraint force. Considering this force in Lagrange-d'Alembert principle is yet another way of obtaining the constrained Euler-Lagrange equations. Here, the forces do not arise as arbitrary external forces, but because the variations δq are not arbitrary elements of $T\mathcal{M}$ but instead they have to be elements of $T\mathcal{N}$. As a consequence some subtleties arise in the discrete setting and special care needs to be taken.

While for the tangent bundle, there exists a canonical embedding of the tangent to the constraint submanifold into the tangent of the ambient manifold, for the cotangent bundle this is not the case and an embedding can only be constructed if there exists a hyper-regular Hamiltonian H . In this case we can construct a symplectic embedding $\eta : T^*\mathcal{N} \rightarrow T^*\mathcal{M}$ covering the embedding $i : \mathcal{N} \rightarrow \mathcal{M}$ by

$$\eta(T^*\mathcal{N}) = \{(x, p) \in T^*\mathcal{M} \mid g(x) = 0, G(x)H_p(x, p) = 0\}. \quad (9.63)$$

The Hamiltonian equivalent of the constrained Euler-Lagrange equations (9.59) are the constrained Hamilton equations,

$$\dot{q} = \frac{\partial H}{\partial p}(q, p), \quad \dot{p} = -\frac{\partial H}{\partial x}(q, p) - \lambda^T \nabla g(q), \quad 0 = g(q). \quad (9.64)$$

In the continuous setting, the Lagrangian as well as the Hamiltonian, the hidden constraint $\dot{q}(q(t)) = 0$ is satisfied automatically. It is an invariant of the flow of (9.59) and (9.64). This will in general be different in the discrete setting, especially for Hamiltonian integrators.

9.3.1 Discrete Action Principle on the Constraint Submanifold

Consider a discrete Lagrangian system $L_d : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R}$ with holonomic constraint $g : \mathcal{M} \rightarrow \mathbb{R}^m$ and corresponding constraint submanifold $\mathcal{N} = g^{-1}(0) \subset \mathcal{M}$. As in the continuous case, the fact that $\mathcal{N} \times \mathcal{N}$ is naturally a submanifold of $\mathcal{M} \times \mathcal{M}$ means that we can restrict the discrete Lagrangian L_d to $\mathcal{N} \times \mathcal{N}$ which we denote by $L_d|_{\mathcal{N} \times \mathcal{N}}$. The discrete action on \mathcal{N} is then given by

$$\mathcal{A}_d|_{\mathcal{N}}[q_d] = \sum_{n=0}^{N-1} L_d|_{\mathcal{N} \times \mathcal{N}}(q_n, q_{n+1}). \quad (9.65)$$

Using the Lagrange multiplier theorem for computing extremal points of $\mathcal{A}_d|_{\mathcal{N}}$ for discrete curves $q_d = \{q_n\}_{n=0}^N$ on \mathcal{N} , we obtain the constrained discrete Euler-Lagrange equations,

$$D_1 L_d(q_n, q_{n+1}) + D_2 L_d(q_{n-1}, q_n) = \lambda_n^T \nabla g(q_n), \quad (9.66a)$$

$$0 = g(q_{n+1}), \quad (9.66b)$$

with the constraint force on the right-hand side of (9.66a) and the discrete constraint in (9.66b).

9.3.2 Variational Integrators for the Augmented Lagrangian

A second way of obtaining the discrete Euler-Lagrange equations with constraints is to extremise the action for the augmented Lagrangian. Here, we have two ways to define the augmented discrete Lagrangian,

$$\bar{L}_d^-(q_n, \lambda_n, q_{n+1}, \lambda_{n+1}) = L_d(q_n, q_{n+1}) - \lambda_n^T g(q_n), \quad (9.67a)$$

$$\bar{L}_d^+(q_n, \lambda_n, q_{n+1}, \lambda_{n+1}) = L_d(q_n, q_{n+1}) - \lambda_{n+1}^T g(q_{n+1}). \quad (9.67b)$$

The corresponding discrete actions,

$$\bar{\mathcal{A}}_d^-[q_d, \lambda_d] = \sum_{n=0}^{N-1} [L_d(q_n, q_{n+1}) - \lambda_n^T g(q_n)], \quad (9.68a)$$

$$\bar{\mathcal{A}}_d^+[q_d, \lambda_d] = \sum_{n=0}^{N-1} [L_d(q_n, q_{n+1}) - \lambda_{n+1}^T g(q_{n+1})], \quad (9.68b)$$

with $q_d = \{q_n\}_{n=0}^N$ a discrete curve in \mathcal{M} and $\lambda_d = \{\lambda_n\}_{n=0}^N$ a discrete curve in \mathbb{R}^m . Both discrete actions have the same extrema as the curves are held fixed at the boundaries. Extremising with respect to q_d gives (9.66a) and extremising with respect to λ_d gives the discrete constraint (9.66b). Alternatively, we could also define the augmented discrete Lagrangian by

$$\bar{L}_d(q_n, \lambda_n, q_{n+1}, \lambda_{n+1}) = L_d(q_n, q_{n+1}) - \frac{1}{2} [\lambda_n^T g(q_n) + \lambda_{n+1}^T g(q_{n+1})]. \quad (9.69)$$

This would still lead to the same set of constrained discrete Euler-Lagrange equations (9.66), so all of the different choices seem to be equivalent. They are, however, not equivalent when it comes to the discrete fibre derivative.

9.3.3 Constrained Discrete Fibre Derivative

Depending on which augmented discrete Lagrangian we consider, we obtain different discrete fibre derivatives, namely for \bar{L}_d^- we obtain

$$\mathbb{F}^- \bar{L}_d^- : (q_n, q_{n+1}) \mapsto (q_n, p_n) = (q_n, -D_1 L_d(q_n, q_{n+1}) + \lambda_n^T \nabla g(q_n)), \quad (9.70a)$$

$$\mathbb{F}^+ \bar{L}_d^- : (q_n, q_{n+1}) \mapsto (q_{n+1}, p_{n+1}) = (q_{n+1}, D_2 L_d(q_n, q_{n+1})), \quad (9.70b)$$

for \bar{L}_d^+ we obtain

$$\mathbb{F}^- \bar{L}_d^+ : (q_n, q_{n+1}) \mapsto (q_n, p_n) = (q_n, -D_1 L_d(q_n, q_{n+1})), \quad (9.71a)$$

$$\mathbb{F}^+ \bar{L}_d^+ : (q_n, q_{n+1}) \mapsto (q_{n+1}, p_{n+1}) = (q_{n+1}, D_2 L_d(q_n, q_{n+1}) - \lambda_{n+1}^T \nabla g(q_{n+1})), \quad (9.71b)$$

and for \bar{L}_d we obtain

$$\mathbb{F}^- \bar{L}_d : (q_n, q_{n+1}) \mapsto (q_n, p_n) = (q_n, -D_1 L_d(q_n, q_{n+1}) + \frac{1}{2} \lambda_n^T \nabla g(q_n)), \quad (9.72a)$$

$$\mathbb{F}^+ \bar{L}_d : (q_n, q_{n+1}) \mapsto (q_{n+1}, p_{n+1}) = (q_{n+1}, D_2 L_d(q_n, q_{n+1}) - \frac{1}{2} \lambda_{n+1}^T \nabla g(q_{n+1})). \quad (9.72b)$$

In all three cases, the corresponding position-momentum form of the integrator is equivalent to the constrained discrete Euler-Lagrange equations (9.66), but there is an important difference. While the map $\tilde{\varphi}_h^-$ corresponding to \bar{L}_d^- and given by

$$p_n = -D_1 L_d(q_n, q_{n+1}) + \lambda_n^T \nabla g(q_n), \quad (9.73a)$$

$$p_{n+1} = D_2 L_d(q_n, q_{n+1}), \quad (9.73b)$$

$$0 = g(q_{n+1}), \quad (9.73c)$$

provides a well-defined forward map, but not a well-defined backward map, the opposite is true for $\tilde{\varphi}_h^+$ corresponding to \bar{L}_d^+ and given by

$$p_n = -D_1 L_d(q_n, q_{n+1}), \quad (9.74a)$$

$$p_{n+1} = D_2 L_d(q_n, q_{n+1}) - \lambda_{n+1}^T \nabla g(q_{n+1}), \quad (9.74b)$$

$$0 = g(q_{n+1}). \quad (9.74c)$$

Only $\tilde{\varphi}_h$, given by

$$p_n = -D_1 L_d(q_n, q_{n+1}) + \frac{1}{2} \lambda_n^T \nabla g(q_n), \quad (9.75a)$$

$$p_{n+1} = D_2 L_d(q_n, q_{n+1}) - \frac{1}{2} \lambda_{n+1}^T \nabla g(q_{n+1}), \quad (9.75b)$$

$$0 = g(q_{n+1}). \quad (9.75c)$$

provides both, a well-defined forward map and a well-defined backward map. But there is another problem. All of these map are taking points $(q_n, p_n) \in \eta(T^*\mathcal{N})$ to points $(q_{n+1}, p_{n+1}) \in T^*\mathcal{M}$. That is, the result of the map is not guaranteed to lie in the cotangent bundle of the constrained submanifold. The reason is, that only the primary constraint is enforced but not the secondary constraint.

To that end, we have to add another projection, enforcing this constraint as well. The constraint force of the secondary constraint has the same form as the one for the primary constraint. In the equation for p_{n+1} we can thus just replace λ_{n+1} with a different multiplier μ_{n+1} and add the secondary constraint, so that the position-momentum form of the constrained discrete Euler-Lagrange equations has the following form,

$$p_n = -D_1 L_d(q_n, q_{n+1}) + \frac{1}{2} \lambda_n^T \nabla g(q_n), \quad (9.76a)$$

$$p_{n+1} = D_2 L_d(q_n, q_{n+1}) - \frac{1}{2} \mu_{n+1}^T \nabla g(q_{n+1}), \quad (9.76b)$$

$$0 = g(q_{n+1}), \quad (9.76c)$$

$$0 = \nabla g(q_{n+1}) \cdot H_p(q_{n+1}, p_{n+1}), \quad (9.76d)$$

defining a map from $(q_n, p_n) \in \eta(T^*\mathcal{N})$ to $(q_{n+1}, p_{n+1}) \in T^*\mathcal{M}$ which will satisfy $(q_{n+1}, p_{n+1}) \in \eta(T^*\mathcal{N})$. Geometrically, this can be justified by requiring the result of the discrete fibre derivative to be an element of the cotangent bundle of \mathcal{N} . To make the connection with the Lagrange multiplier theorem, we define the discrete fibre derivative via its contraction with an element of the tangent bundle of \mathcal{N} .

9.3.4 SHAKE and RATTLE

We had seen before that the Verlet algorithm is the variational integrator corresponding to the trapezoidal discretisation of the Lagrangian,

$$L_d^{\text{tr}}(q_n, q_{n+1}) = \frac{h}{2} L\left(q_n, \frac{q_{n+1} - q_n}{h}\right) + \frac{h}{2} L\left(q_{n+1}, \frac{q_{n+1} - q_n}{h}\right), \quad (9.77)$$

where we assumed that the continuous Lagrangian has the form

$$L(q, \dot{q}) = \frac{1}{2} \dot{q}^T M \dot{q} - U(q). \quad (9.78)$$

A constrained version of the method is obtained simply by restricting the discrete Lagrangian L_d to $\mathcal{N} \times \mathcal{N}$ and calculating the constrained discrete Euler-Lagrange equations (9.66). These give

$$M \left(\frac{q_{n+1} - 2q_n + q_{n-1}}{h^2} \right) + \nabla U(q_n) + \lambda_n^T \nabla g(q_n) = 0, \quad (9.79a)$$

$$g(q_{n+1}) = 0, \quad (9.79b)$$

which is known as the SHAKE algorithm. The position-momentum form (9.76) of this Lagrangian,

$$\begin{aligned} p_n &= M \frac{q_{n+1} - q_n}{h} + \frac{1}{2} \nabla U(q_n) + \frac{1}{2} \lambda_n^T \nabla g(q_n), \\ p_{n+1} &= M \frac{q_{n+1} - q_n}{h} - \frac{1}{2} \nabla U(q_{n+1}) - \frac{1}{2} \mu_{n+1}^T \nabla g(q_{n+1}), \\ 0 &= g(q_{n+1}), \\ 0 &= G(q_{n+1}) M^{-1} p_{n+1}. \end{aligned} \quad (9.80)$$

which upon introducing $p_{n+1/2}$ as defined below leads us to the RATTLE algorithm, which reads

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2} [\nabla U(q_n) + \lambda_n^T \nabla g(q_n)], \\ q_{n+1} &= q_n + h M^{-1} p_{n+1/2}, \\ 0 &= g(q_{n+1}), \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2} [\nabla U(q_{n+1}) + \mu_{n+1}^T \nabla g(q_{n+1})], \\ 0 &= G(q_{n+1}) M^{-1} p_{n+1}. \end{aligned} \quad (9.81)$$

The general formulation on the Hamiltonian side is given by

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2} [H_x(q_n, p_{n+1/2}) + \nabla g(q_n)^T \lambda_{n+1}], \\ q_{n+1} &= q_n + \frac{h}{2} [H_p(q_n, p_{n+1/2}) + H_p(q_{n+1}, p_{n+1/2})], \\ 0 &= g(q_{n+1}), \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2} [H_x(q_{n+1}, p_{n+1/2}) + \nabla g(q_n)^T \mu_{n+1}], \\ 0 &= G(q_{n+1}) H_p(q_{n+1}, p_{n+1}). \end{aligned} \quad (9.82)$$

This shows that both the SHAKE and the RATTLE algorithm can be derived from a discrete Lagrangian.

9.3.5 Constrained Variational Runge-Kutta Methods

For a Hamiltonian system $H : T^*\mathcal{M}$ with holonomic constraint $g : \mathcal{M} \rightarrow \mathbb{R}^m$, a constrained partitioned Runge-Kutta method is a map $T^*\mathcal{M} \rightarrow T^*\mathcal{M}$ defined by

$$q_{n+1} = q_n + h \sum_{i=1}^s b_i \dot{Q}_{n,i}, \quad p_{n+1} = p_n + h \sum_{i=1}^s \bar{b}_i \dot{P}_{n,i}, \quad (9.83a)$$

$$Q_{n,i} = q_n + h \sum_{j=1}^s a_{ij} \dot{Q}_{n,j}, \quad P_{n,j} = p_n + h \sum_{i=1}^s \bar{a}_{ij} \dot{P}_{n,i}, \quad (9.83b)$$

$$\dot{Q}_{n,i} = \frac{\partial H}{\partial p}(Q_{n,i}, P_{n,i}), \quad \dot{P}_{n,i} = -\frac{\partial H}{\partial x}(Q_{n,i}, P_{n,i}) - \Lambda_i^T \nabla g(Q_i), \quad (9.83c)$$

$$0 = g(Q_{n,i}), \quad 0 = \nabla g(q_{n+1}) \cdot \frac{\partial H}{\partial p}(q_{n+1}, p_{n+1}), \quad (9.83d)$$

with

$$b_i \bar{a}_{ij} + \bar{b}_j a_{ji} = b_i \bar{b}_j, \quad \bar{b}_i = b_i. \quad (9.84)$$

In order for this integrator to have a solution, i.e., not to be over-determined, we have to require that $Q_{n,1} = q_n$, and to ensure that this solution is in $T^*\mathcal{M}$ we also have to require that $Q_{n,s} = q_{n+1}$.

9.3.6 Discrete Lagrange-d'Alembert Principle

In the discussion about the discrete fibre derivatives, it did not become entirely clear why any of the augmented discrete Lagrangians should be preferable over the others. We had seen that the application of the constraints results in an additional force $F = \lambda^T \nabla g(q)$ being added to the system. From our previous discussion, we should expect that we can add this force via the Lagrange-d'Alembert principle, with the forces consistently discretised in the same as as the Lagrangian. In general, however, this will not lead to the constraint being enforced and satisfied at q_{n+1} . We have just seen with the constrained Runge-Kutta methods that we have to require that the last internal stage corresponds to the solution at the next time step, exactly for this reason. Thus some care needs to be taken when applying the discrete Lagrange-d'Alembert principle in order to enforce constraints. We will come back to this issue in the discussion on nonholonomic constraints.

9.4 Nonholonomic Constraints

In contrast to holonomic constraints, nonholonomic constraints are also allowed to depend on the velocities, that is they are specified by some function $g(q, \dot{q}) = 0$. We will focus on linear constraints, which have the form

$$g^a(q, \dot{q}) = \mu_i^a(q) \dot{q}^i = 0, \quad 1 \leq a \leq m. \quad (9.85)$$

These cover most physical systems of interest. The constraints define a constraint submanifold, often referred to as distribution, $\mathcal{D} \subset T\mathcal{M}$, given by

$$\mathcal{D} = \{(x, v) \in T\mathcal{M} \mid g(x, v) = 0\}. \quad (9.86)$$

For a given Lagrangian $L : T\mathcal{M} \rightarrow \mathbb{R}$ the following Lagrange-d'Alembert principle provides the equations of motion.

Definition 9.7. The Lagrange-d'Alembert equations of motion for the system with Lagrangian L and constraint distribution \mathcal{D} are those determined by

$$\delta \int_{t_1}^{t_2} L(q(t), \dot{q}(t)) dt = 0, \quad (9.87)$$

where the variations $\delta q(t)$ of the curve $q(t)$ are required to satisfy the constraint for each $t \in [t_1, t_2]$ and vanish at the endpoints, i.e., $\delta q(t_1) = \delta q(t_2) = 0$. In addition, the curve itself is required to satisfy the constraints, that is $(q, \dot{q}) \in \mathcal{D}$.

Remark 9.8. Note that in the above definition, variations are taken before imposing the constraints. That is, the constraints are not imposed on the family of curves defining the variation. These operation do not commute, and this fact is central to the fact that nonholonomic mechanics is nonvariational.

The Lagrange-d'Alembert principle is equivalent to the equations

$$\delta L = \left[\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{v}}(q(t), \dot{q}(t)) \right) - \frac{\partial L}{\partial x}(q(t), \dot{q}(t)) \right] \cdot \delta q = 0, \quad (9.88)$$

for all variations δq satisfying the constraints at each point of the underlying curve $q(t)$, i.e., such that $\mu_i^\alpha(q) \delta q^i = 0$. This leads to the equations

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{v}^i}(q(t), \dot{q}(t)) \right) - \frac{\partial L}{\partial x^i}(q(t), \dot{q}(t)) = \sum_{a=1}^m \lambda_a(t) \mu_i^\alpha(q(t)), \quad 1 \leq i \leq d, \quad (9.89)$$

where the right-hand side defines the constraint force $F_L = \lambda^T \mu(q)$.

9.4.1 Discrete Lagrange-d'Alembert Principle

Let us consider a discrete constraint space $\mathcal{D}_d \subset \mathcal{M} \times \mathcal{M}$ with the same dimension as \mathcal{M} and such that $(x, x) \in \mathcal{D}_d$ for all $x \in \mathcal{M}$. The particular choice of \mathcal{D}_d is important in order to obtain a consistent discretisation of the continuous equations of motion. More specifically, the discrete Lagrangian $L_d : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R}$ and the discrete constraint space \mathcal{D}_d should be selected in a consistent way. That is, one uses the same type of discretisation for the Lagrangian $L : T\mathcal{M} \rightarrow \mathbb{R}$ and the constraint functions $g : T\mathcal{M} \rightarrow \mathbb{R}^m$. For instance, if L_d is constructed by means of a discretisation mapping $\Psi : \mathcal{M} \times \mathcal{M} \rightarrow T\mathcal{M}$, that is $L_d = L \circ \Psi$, then \mathcal{D}_d must locally be defined by the annihilation of the function $g_d = g \circ \Psi$.

In order to define the discrete Lagrange-d'Alembert principle, we need three ingredients: a discrete Lagrangian L_d , a constraint distribution \mathcal{D} and the discrete constraint space \mathcal{D}_d . Then the discrete Lagrange-d'Alembert principle corresponds to the extremisation of

$$\sum_{n=0}^{N-1} L_d(q_n, q_{n+1}), \quad (9.90)$$

on the discrete trajectory $q_d = \{q_n\}_{n=0}^N$ with fixed endpoints q_0 and q_N , where the variations must satisfy $\delta q_n \in \mathcal{D}_{q_n}$ and for each pair of points $(q_n, q_{n+1}) \in \mathcal{D}_d$. Thus leads to the set of equations

$$\left[D_1 L_d(q_n, q_{n+1}) + D_2 L_d(q_{n-1}, q_n) \right] \cdot \delta q_n = 0. \quad (9.91)$$

If $g_d : \mathcal{M} \times \mathcal{M} \rightarrow \mathbb{R}^m$ is a vector-valued function whose annihilation defines \mathcal{D}_d , we obtain the following discrete Lagrange-d'Alembert algorithm,

$$D_1 L_d(q_n, q_{n+1}) + D_2 L_d(q_{n-1}, q_n) = \lambda_n^T \mu(q_n), \quad (9.92a)$$

$$g_d(q_n, q_{n+1}) = 0. \quad (9.92b)$$

As an example, consider the following discrete Lagrangian

$$L_d^\alpha(q_n, q_{n+1}) = h L\left((1 - \alpha) q_n + \alpha q_{n+1}, \frac{q_{n+1} - q_n}{h}\right), \quad (9.93a)$$

for some parameter $\alpha \in [0, 1]$. The natural discrete constraint for this Lagrangian is

$$g_d(q_n, q_{n+1}) = g\left((1 - \alpha) q_n + \alpha q_{n+1}, \frac{q_{n+1} - q_n}{h}\right). \quad (9.93b)$$

9.4.2 Nonholonomic SHAKE and RATTLE

The nonholonomic versions of SHAKE and RATTLE are given by

$$M\left(\frac{q_{n+1} - 2q_n + q_{n-1}}{h^2}\right) + \nabla U(q_n) + \lambda_n^T \mu(q_n) = 0, \quad (9.94a)$$

$$\mu(q_n) \cdot \frac{q_{n+1} - q_{n-1}}{2h} = 0, \quad (9.94b)$$

and by

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2} [\nabla U(q_n) + \lambda_n^T \mu(q_n)], \\ q_{n+1} &= q_n + h M^{-1} p_{n+1/2}, \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2} [\nabla U(q_{n+1}) + \lambda_{n+1}^T \mu(q_{n+1})], \\ 0 &= \mu(q_{n+1}) M^{-1} p_{n+1}, \end{aligned} \quad (9.95)$$

respectively.

9.4.3 SPARK Methods

The idea of special partitioned additive Runge-Kutta (SPARK) methods is to approximate the exact discrete Lagrangian and the constraint force differently. They lead to the following general scheme,

$$q_{n+1} = q_n + h \sum_{i=1}^s b_i \dot{Q}_{n,i}, \quad p_{n+1} = p_n + h \sum_{i=1}^s \bar{b}_i \dot{P}_{n,i} - h \sum_{i=1}^{\tilde{s}} \tilde{b}_i \Lambda_i^T \mu(\tilde{Q}_i), \quad (9.96a)$$

$$Q_{n,i} = q_n + h \sum_{j=1}^s a_{ij} \dot{Q}_{n,j}, \quad P_{n,j} = p_n + h \sum_{i=1}^s \bar{a}_{ij} \dot{P}_{n,i} - h \sum_{j=1}^{\tilde{s}} \tilde{a}_{ij} \Lambda_j^T \mu(\tilde{Q}_j), \quad (9.96b)$$

$$\tilde{Q}_{n,i} = q_n + h \sum_{j=1}^s \alpha_{ij} \dot{Q}_{n,j}, \quad \tilde{P}_{n,i} = p_n + h \sum_{j=1}^s \bar{\alpha}_{ij} \dot{P}_{n,j} - h \sum_{j=1}^{\tilde{s}} \tilde{\alpha}_{ij} \Lambda_j^T \mu(\tilde{Q}_j), \quad (9.96c)$$

$$\dot{Q}_{n,i} = \frac{\partial H}{\partial p}(Q_{n,i}, P_{n,i}), \quad \dot{P}_{n,i} = -\frac{\partial H}{\partial x}(Q_{n,i}, P_{n,i}), \quad (9.96d)$$

$$0 = \mu(q_{n+1}) \cdot \frac{\partial H}{\partial p}(q_{n+1}, p_{n+1}), \quad 0 = \sum_{j=1}^{\tilde{s}} \mu(\tilde{Q}_{n,j}) \cdot \frac{\partial H}{\partial p}(\tilde{Q}_{n,j}, \tilde{P}_{n,j}), \quad (9.96e)$$

with symplecticity conditions

$$\bar{b}_i a_{ij} + b_j \bar{a}_{ji} = \bar{b}_i b_j, \quad \bar{b}_i \tilde{a}_{ij} + \tilde{b}_j \bar{a}_{ji} = \bar{b}_i \tilde{b}_j, \quad \bar{b}_i = b_i. \quad (9.97)$$

The matrix ω depends on the underlying Runge-Kutta methods. For Gauss-Legendre methods, ω_{ij} can be taken as $\omega_{ij} = \tilde{b}_j \tilde{c}_j^{i-1}$ for $i = 1, \dots, \tilde{s} - 1$ and $j = 1, \dots, \tilde{s}$.

9.5 Dirac Constraints

Dirac constraints (or primary constraints in the sense of Dirac) arise in problems with degenerate Lagrangian, that is a Lagrangian for which

$$\frac{\partial^2 L}{\partial v^i \partial v^j} = 0$$

for some or all i, j . Examples of such systems include certain Lotka-Volterra systems used in population dynamics, reduced charged particle models of plasma physics, and planar point vortices.

9.5.1 Degenerate Lagrangian Systems

Let us consider degenerate Lagrangian systems

$$L : \mathcal{T}\mathcal{M} \rightarrow \mathbb{R}, \quad (9.98)$$

whose Lagrangian L is linear in velocities, in particular systems of the form

$$L(q, \dot{q}) = \langle \alpha(q), \dot{q} \rangle - H(q), \quad (9.99)$$

where α is a general, possibly nonlinear function of q . The Euler-Lagrange equations for this Lagrangian read

$$\nabla \alpha(q) \cdot \dot{q} - \nabla H(q) - \frac{d}{dt} \alpha(q) = 0, \quad (9.100)$$

which after computing the time-derivative of α becomes

$$\bar{\Omega}^T(q) \dot{q} = \nabla H(q), \quad (9.101)$$

with $\bar{\Omega}$ the noncanonical symplectic matrix on \mathcal{M} , given by

$$\bar{\Omega}_{ij}(q) = \alpha_{i,j}(q) - \alpha_{j,i}(q). \quad (9.102)$$

Note that $\bar{\Omega}$ is not the symplectic matrix Ω_L on $\mathcal{T}\mathcal{M}$ originating from the boundary terms in the action principle. As the Lagrangian (9.99) is degenerate, so is the corresponding symplectic matrix Ω_L , which can be written in block matrix form as

$$\Omega_L = \begin{pmatrix} \bar{\Omega} & 0 \\ 0 & 0 \end{pmatrix}, \quad (9.103)$$

where the upper left block corresponds to the noncanonical symplectic matrix $\bar{\Omega}$ on \mathcal{M} . When we discuss symplecticity in the following, we are always referring to the noncanonical symplectic matrix $\bar{\Omega}$.

9.5.2 Dirac Constraints

Degenerate systems of the form (9.99) can also be treated as a canonical Hamiltonian system (q, p) on the cotangent bundle $T^*\mathcal{M}$, subject to a primary constraint in the sense of Dirac, namely

$$g(q, p) = p - \alpha(q) = 0, \quad (9.104)$$

originating from the Legendre transform,

$$p = \frac{\partial L}{\partial v}(q, \dot{q}) = \alpha(q). \quad (9.105)$$

That is, the dynamics is restricted to the distribution

$$\Delta = \{(q, p) \in T^*Q \mid g(q, p) = 0\} \subset T^*Q. \quad (9.106)$$

The equations of motion for this system can be derived from the phasespace action

$$\bar{\mathcal{A}}[q, p] = \int [\langle p, \dot{q} \rangle - \bar{H}(q, p, \lambda)] dt, \quad (9.107)$$

with the augmented Hamiltonian \bar{H} defined as

$$\bar{H}(q, p, \lambda) = H(q) + g^T(q, p) \lambda. \quad (9.108)$$

Applying Hamilton's action principle to (9.107) results in the following index two differential-algebraic system of equations,

$$\dot{q} = H_p(q) + \lambda^T g_p(q, p), \quad (9.109a)$$

$$\dot{p} = -H_x(q) - \lambda^T g_x(q, p), \quad (9.109b)$$

$$0 = g(q, p). \quad (9.109c)$$

With $z = (p, q)$, this can be rewritten as

$$\dot{z} = f(z, \lambda), \quad (9.110a)$$

$$0 = g(z), \quad (9.110b)$$

where

$$f(z, \lambda) = \Omega^{-1} \nabla H(z) + \Omega^{-1} \lambda^T \nabla g(z), \quad (9.110c)$$

∇ denotes the derivatives with respect to z , and Ω is the canonical symplectic matrix on $T^*\mathcal{M}$, given by

$$\Omega = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}. \quad (9.111)$$

Preserving the canonical symplectic form $\omega = \frac{1}{2} \Omega_{ij} dx^i \wedge dp^j$ as well as the constraint g implies preservation of the noncanonical symplectic matrix $\bar{\omega}(q) = \frac{1}{2} \bar{\Omega}(q) dx^i \wedge dx^j$.

9.5.3 Symplecticity

Our aim is to construct methods which retain the symplecticity of the integrator as well as its momentum maps. Care has to be taken, when stating that the variational integrator and the projection are symplectic. The continuous system preserves two symplectic forms, the canonical two-form ω on $T^*\mathcal{M}$, but also the noncanonical two-form $\bar{\omega}(q)$ on \mathcal{M} , given by

$$\bar{\omega} = d\alpha = \frac{1}{2} \bar{\Omega}_{ij} dx^i \wedge dx^j, \quad (9.112)$$

with components

$$\bar{\Omega}_{ij} = \frac{\partial \alpha_j}{\partial x^i} - \frac{\partial \alpha_i}{\partial x^j}. \quad (9.113)$$

As by the constraint $p_i = \alpha_i(q)$, we have

$$dp_i = \frac{\partial \alpha_i}{\partial x^j} dx^j, \quad (9.114)$$

and

$$\begin{aligned} \omega = dp_i \wedge dq^i &= \frac{\partial \alpha_i}{\partial x^j} dx^j \wedge dx^i = \frac{1}{2} \frac{\partial \alpha_i}{\partial x^j} dx^j \wedge dx^i + \frac{1}{2} \frac{\partial \alpha_j}{\partial x^i} dx^i \wedge dx^j \\ &= \frac{1}{2} \left(\frac{\partial \alpha_j}{\partial x^i} - \frac{\partial \alpha_i}{\partial x^j} \right) dx^i \wedge dx^j = \bar{\omega}. \end{aligned} \quad (9.115)$$

The noncanonical two-form is the one of interest. However, assuming that the constraint $\phi(q, p) = 0$ is satisfied, the canonical symplectic form on $T^*\mathcal{M}$ reduces to the noncanonical one on \mathcal{M} . So it suffices to show that the canonical symplectic form Ω on $T^*\mathcal{M}$ is preserved.

9.5.4 Discretisation

In order to discretise this system, we can follow several paths, most of which will not lead to success. One option is to directly discretise the degenerate Lagrangian (9.99) and compute the corresponding discrete Euler-Lagrange equations, e.g., for the trapezoidal and midpoint discretisation,

$$\nabla \alpha(q_n) \cdot \frac{q_{n+1} - q_{n-1}}{2h} - \frac{\alpha(q_{n+1}) - \alpha(q_{n-1})}{2h} - \nabla H(q_n) = 0, \quad (9.116)$$

and

$$\begin{aligned} \frac{1}{2} \nabla \alpha(q_{n+1/2}) \cdot \frac{q_{n+1} - q_n}{h} + \frac{1}{2} \nabla \alpha(q_{n-1/2}) \cdot \frac{q_n - q_{n-1}}{h} - \frac{\alpha(q_{n+1/2}) - \alpha(q_{n-1/2})}{h} \\ - \frac{1}{2} (\nabla H(q_{n+1/2}) + \nabla H(q_{n-1/2})) = 0, \end{aligned} \quad (9.117)$$

respectively, where $q_{n+1/2} = \frac{1}{2}(q_n + q_{n+1})$, or the discrete position-momentum form,

$$\dots \quad (9.118)$$

and

$$\dots \quad (9.119)$$

respectively. In the former case, we obtain a multistep method that is susceptible to parasitic modes. In the latter case, we find that the resulting integrator will not satisfy the constraint (9.104) unless α is a linear function of q , that is the solution will drift away from the constraint submanifold (9.106).

Another option is to discretise the phasespace action (9.107). This will enforce the constraint, but for values of q and p at different times, e.g., $\phi(q_n, p_{n+1}) = 0$, which is not meaningful, so that the solution will still drift away from the constraint submanifold. The natural framework for degenerate Lagrangian systems is the Hamilton-Pointryagin principle,

$$\mathcal{A} = \int [L(q, \lambda) + \langle p, \dot{q} - \lambda \rangle]. \quad (9.120)$$

Here, the constraint $p = \alpha(q)$ naturally appears as one of the equations of motion. However, it is not hard to see that this formulation is equivalent to the phasespace action (9.107). Therefore a discrete version of the Hamilton-Pointryagin principle will lead to exactly the same problems.

Interestingly, if we derive variational Runge-Kutta methods for the phasespace Lagrangian (9.107) or the Hamilton-Pontryagin action (9.120), say Gauss-Legendre methods, we find that the constraints are automatically satisfied for the internal stages of the Runge-Kutta method but not for the final step. This is due to the fact that the internal stages obey discrete versions of the equations of motion, whereas the final step merely amounts to a numerical quadrature.

Below we sketch only the first of these possibilities, followed by a discussion on how projection methods can be used to enforce the constraint at the final step, i.e., $\phi(q_{n+1}, p_{n+1}) = 0$. That is, we take the solution of a variational integrator and project it to the constraint submanifold (9.106).

10 Lagrangian Field Theory

In the infinite dimensional case (field theory), the Lagrangian can in principle depend on the fields, their derivatives, and also the coordinates. In many applications, however, the latter is not the case, hence for simplicity it is not considered here. The right geometric framework for Lagrangian and Hamiltonian field theories is that of jet bundles, where the general case can be treated without further complications.

With the restriction to Lagrangians that are only functions of the fields and their first derivatives, the derivation of Hamilton's action principle is not any more complicated than in the finite dimensional case (particle mechanics). Without loss of generality, consider as base space \mathcal{X} only time plus one spatial dimension (t, x) and a theory of just one scalar field $\varphi(t, x)$. The Lagrangian density is thus a function

$$\mathcal{L} = \mathcal{L}(\varphi(t, x), \varphi_t(t, x), \varphi_x(t, x)), \quad (10.1)$$

and the action is given by

$$\mathcal{A}[\varphi] = \int_{\mathcal{X}} \mathcal{L}(\varphi, \varphi_t, \varphi_x) = \int_{\mathcal{X}} L(\varphi, \varphi_t, \varphi_x) dt dx. \quad (10.2)$$

For instructive reasons, all considerations in this section will be taken with respect to the Lagrangian function L . Consider a family of variations φ^ϵ of φ that is defined by

$$\varphi^\epsilon(t, x) = \varphi(t, x, \epsilon) \quad \text{with} \quad \varphi^0 = \varphi(t, x). \quad (10.3)$$

The variation of the action can be expressed as

$$\left. \frac{d}{d\epsilon} \mathcal{A}[\varphi^\epsilon] \right|_{\epsilon=0} = \frac{d}{d\epsilon} \left[\int_{\mathcal{X}} L(\varphi^\epsilon(t, x), \varphi_t^\epsilon(t, x), \varphi_x^\epsilon(t, x)) dt dx \right]_{\epsilon=0}, \quad (10.4)$$

and Hamilton's principle of stationary action states that φ is a critical point of the action if and only if (10.4) vanishes for all variations φ^ϵ of φ . The differentiation is carried out under the integral to give

$$\left. \frac{d}{d\epsilon} \mathcal{A}[\varphi^\epsilon] \right|_{\epsilon=0} = \int_{\mathcal{X}} \left[\frac{dL}{d\epsilon}(\varphi^\epsilon, \varphi_t^\epsilon, \varphi_x^\epsilon) \right]_{\epsilon=0} dt dx \quad (10.5)$$

$$= \int_{\mathcal{X}} \left[\frac{\partial L}{\partial \varphi} \frac{\partial \varphi^\epsilon}{\partial \epsilon} + \frac{\partial L}{\partial \varphi_t} \frac{\partial \varphi_t^\epsilon}{\partial \epsilon} + \frac{\partial L}{\partial \varphi_x} \frac{\partial \varphi_x^\epsilon}{\partial \epsilon} \right]_{\epsilon=0} dt dx. \quad (10.6)$$

The second and third term are integrated by parts with respect to t and x , respectively,

$$\left. \frac{d}{d\epsilon} \mathcal{A}[\varphi^\epsilon] \right|_{\epsilon=0} = \int_{\mathcal{X}} \left[\frac{\partial L}{\partial \varphi} - \frac{\partial}{\partial t} \frac{\partial L}{\partial \varphi_t} - \frac{\partial}{\partial x} \frac{\partial L}{\partial \varphi_x} \right] \frac{\partial \varphi^\epsilon}{\partial \epsilon} \Big|_{\epsilon=0} dt dx, \quad (10.7)$$

where it is assumed that the fields vanish at infinity such that the boundary terms vanish. Except for this restriction, the functions $\partial_\epsilon \varphi^\epsilon$ are arbitrary, such that the variation of the action vanishes, iff the expression in square brackets vanishes, which is what now leads to the Euler-Lagrange field equations in one spatial dimension,

$$\frac{\partial L}{\partial \varphi} - \frac{\partial}{\partial t} \frac{\partial L}{\partial \varphi_t} - \frac{\partial}{\partial x} \frac{\partial L}{\partial \varphi_x} = 0. \quad (10.8)$$

As expected, there were no surprises and the derivation was very similar to the one of the finite dimensional case, presented in Chapter 4. The usual notation is retained by identifying

$$\delta \varphi = \left. \frac{d}{d\epsilon} \varphi^\epsilon \right|_{\epsilon=0}, \quad (10.9)$$

such that the variation of the action reads

$$\delta \mathcal{A}[\varphi] = \int_{\mathcal{X}} \delta L(\varphi^\epsilon, \varphi_t^\epsilon, \varphi_x^\epsilon) dt dx, \quad (10.10)$$

and the usual manipulations amount to

$$\begin{aligned} \delta \mathcal{A}[\varphi] &= \int_{\mathcal{X}} \left[\frac{\partial L}{\partial \varphi} \delta \varphi + \frac{\partial L}{\partial \varphi_t} \delta \varphi_t + \frac{\partial L}{\partial \varphi_x} \delta \varphi_x \right] dt dx \\ &= \int_{\mathcal{X}} \left[\frac{\partial L}{\partial \varphi} - \frac{\partial}{\partial t} \frac{\partial L}{\partial \varphi_t} - \frac{\partial}{\partial x} \frac{\partial L}{\partial \varphi_x} \right] \delta \varphi dt dx, \end{aligned} \quad (10.11)$$

with the term in square brackets corresponding to the Euler-Lagrange field equations (10.8).

Example: The Wave Equation

Consider the following Lagrangian,

$$L(u_t(t, x), u_x(t, x)) = \frac{1}{2} \left(\frac{\partial u}{\partial t}(t, x) \right)^2 - \frac{1}{2} \left(\frac{\partial u}{\partial x}(t, x) \right)^2. \quad (10.12)$$

Computing the Euler-Lagrange field equations (10.8), we get

$$-\frac{\partial}{\partial t} \left(\frac{\partial u}{\partial t}(t, x) \right) + \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x}(t, x) \right) = 0, \quad (10.13)$$

hence we obtain the linear wave equation,

$$\frac{\partial^2 u}{\partial t^2}(t, x) - \frac{\partial^2 u}{\partial x^2}(t, x) = 0. \quad (10.14)$$

10.1 Dynamics on Jet Bundles

The appropriate geometric setting for Lagrangian field theory is that of jet bundle theory.¹ Rewriting the theory in this framework might at first sight seem to unnecessarily complicate things, but its great advantage is that it offers a concise notation that readily generalises to the case of field theories. That way, jet bundle theory offers a general formulation of the variational problem that applies to finite as well as infinite dimensional systems. Besides, this formulation is fully covariant, the analysis of symmetries with Noether's theorem is simpler, and it resembles the discrete setting quite nicely.

The idea of a jet is to combine the independent variables (coordinates), the dependent variables (trajectories, fields) and their partial derivatives up to a given order in one single geometric object. Jets provide a coordinate-free description of differential equations, which is especially useful in the theory of partial differential equations, where they allow us to represent an infinite-dimensional space of maps by sections of a finite dimensional space of jets, thereby avoiding the intricacies of infinite dimensional manifolds.

Consider a function $\varphi(x)$. It establishes a correspondence between each value $x \in \mathcal{X}$ and another value $\varphi(x) \in \mathcal{F}$. This second value $\varphi(x)$ can be considered as a point in the fibre \mathcal{F} above x . So it seems natural to construct a fibre bundle \mathcal{Y} over the base manifold \mathcal{X} with fibres corresponding to \mathcal{F} . In other words, \mathcal{Y} is obtained by attaching a fibre \mathcal{F} to each point $x \in \mathcal{X}$, such that the fibres of \mathcal{Y} contain all possible values of functions $\varphi(x)$, which can therefore be considered as sections φ in the bundle \mathcal{Y} ,

$$\varphi : \mathcal{X} \rightarrow \mathcal{Y} \quad \text{with} \quad \pi_{\mathcal{X}\mathcal{Y}} \circ \varphi = \text{id}_{\mathcal{X}}, \quad (10.15)$$

where $\pi_{\mathcal{X}\mathcal{Y}}$ is the canonical projection

$$\pi_{\mathcal{X}\mathcal{Y}} : \mathcal{Y} \rightarrow \mathcal{X}. \quad (10.16)$$

If (x^μ, y^a) are coordinates on \mathcal{Y} , a section φ is a map $x \mapsto (x^\mu, \varphi^a(x))$, where we denote by φ^a the vertical components of φ , i.e., the fibre coordinates of $\varphi(x)$. In this setting, the equivalent to the tangent bundle is the first jet bundle $J^1\mathcal{Y}$, which contains the first order partial derivatives of each section $\varphi \in \mathcal{Y}$. In the same way, the k th jet bundle $J^k\mathcal{Y}$ of \mathcal{Y} is the space that contains the partial derivatives of each section $\varphi \in \mathcal{Y}$ up to order k . However, in what follows only the first order jet bundle $J^1\mathcal{Y}$ is needed, so all considerations are restricted to that case.

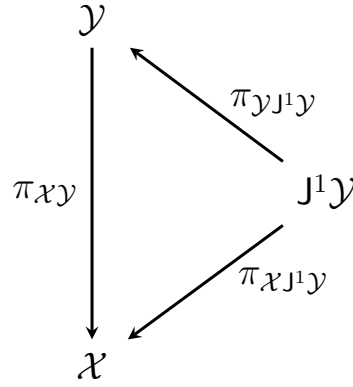
Coordinates on $J^1\mathcal{Y}$ are (x^μ, y^a, v_μ^a) , where x^μ are the coordinates of the base manifold \mathcal{X} , y^a are the values of fields at x , and v_μ^a are all possible values of the partial derivative of y^a with respect to x^μ . $J^1\mathcal{Y}$ has two natural projections. It can be viewed as a fibre bundle over \mathcal{X} with the source projection

$$\pi_{\mathcal{X}, J^1\mathcal{Y}} : J^1\mathcal{Y} \rightarrow \mathcal{X} \quad (10.17)$$

as well as a fibre bundle over \mathcal{Y} with the target projection

$$\pi_{\mathcal{Y}, J^1\mathcal{Y}} : J^1\mathcal{Y} \rightarrow \mathcal{Y}. \quad (10.18)$$

¹The derivations of this section follow along the lines of Gotay, Isenberg, and Marsden [29], Marsden, Patrick, and Shkoller [53, 57], Kouranbaeva and Shkoller [45], Kouranbaeva [44] and West [78].



The first point of view is especially important. Consider a section $\varphi : \mathcal{X} \rightarrow \mathcal{Y}$ of $\pi_{\mathcal{X}\mathcal{Y}}$. Its tangent map $T_x\varphi$ at $x \in \mathcal{X}$ is represented by the matrix $\partial\varphi^a(x)/\partial x^\mu = \varphi_\mu^a(x)$ and thus can be identified with an element of $J^1_{\varphi(x)}\mathcal{Y}$. The map $x \mapsto T_x\varphi$ is therefore a section of $\pi_{\mathcal{X},J^1\mathcal{Y}}$, i.e., a section of $J^1\mathcal{Y}$ regarded as a bundle over \mathcal{X} . This section, denoted $j^1\varphi$, is called the *first jet prolongation*² (also *canonical prolongation*) of a section $\varphi(x)$,

$$j^1\varphi : \mathcal{X} \rightarrow J^1\mathcal{Y} \quad \text{in coordinates} \quad j^1\varphi : x \mapsto (x^\mu, \varphi^a(x), \varphi_\mu^a(x)). \quad (10.19)$$

Such sections $j^1\varphi$ of $J^1\mathcal{Y}$ that correspond to the canonical prolongation³ of a section $\varphi \in \mathcal{Y}$ are called *holonomic*. For them v_μ^a can be identified with $\varphi_\mu^a = \partial\varphi^a/\partial x^\mu$.

In this setting, a section $j^1\varphi$ of $\pi_{\mathcal{X},J^1\mathcal{Y}}$ generalises the notion of a trajectory and a field. The *Lagrangian density* \mathcal{L} is a n -form on the jet bundle $J^1\mathcal{Y}$,

$$\mathcal{L} : J^1\mathcal{Y} \rightarrow \Omega^n(\mathcal{X}), \quad (10.20)$$

where $\Omega^n(\mathcal{X})$ denotes the n -forms on \mathcal{X} . The Lagrangian L is a function on the jet bundle $J^1\mathcal{Y}$,

$$L : J^1\mathcal{Y} \rightarrow \mathbb{R}. \quad (10.21)$$

The connection between the two is drawn by the volume form ω of the base manifold \mathcal{X} ,

$$\mathcal{L} = L\omega. \quad (10.22)$$

Here, n is the dimension of the base space \mathcal{X} and $\omega = dx^1 \wedge dx^2 \wedge \dots \wedge dx^n$, e.g., for \mathcal{X} corresponding to spacetime we have $\omega = dt \wedge dx \wedge dy \wedge dz$.

Hamilton's Action Principle on the Jet Bundle

In the framework of jet bundles, the action is given as the integral of the pullback of the Lagrangian density \mathcal{L} with the first jet prolongation $j^1\varphi$ of a section $\varphi : \mathcal{X} \rightarrow \mathcal{Y}$

$$\mathcal{A}[\varphi] = \int_{\mathcal{X}} (j^1\varphi)^* \mathcal{L}. \quad (10.23)$$

²The jet prolongation can be seen as producing a coordinate-free Taylor expansion to first (in general k th) order, as the jet bundle $J^1\mathcal{Y}$ contains all functions that have the same Taylor series up to the first term.

³Not all sections of $J^1\mathcal{Y}$ are prolongations of a section $\varphi \in \mathcal{Y}$.

As $\mathcal{L} = L\omega$ and L is a smooth function, the following expressions are equivalent

$$(j^1\varphi)^*\mathcal{L} = L(j^1\varphi)\omega. \quad (10.24)$$

Writing the action (10.23) with respect to the last expression and in coordinates

$$\mathcal{A}[\varphi] = \int_{\mathcal{X}} L(j^1\varphi)\omega = \int_{\mathcal{X}} L(x^\mu, \varphi^a, \varphi_\mu^a)\omega \quad (10.25)$$

establishes a correspondence between (10.23) and previous formulation (??). Hamilton's principle states that φ is a critical point of the action iff

$$\left. \frac{d}{d\epsilon} \mathcal{A}[\varphi_\epsilon] \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} \left[\int_{\mathcal{X}} (j^1\varphi_\epsilon)^*\mathcal{L} \right] \right|_{\epsilon=0} = 0 \quad (10.26)$$

for all variations φ_ϵ of φ . These variations are defined as a composition of the trajectory φ and the vertical transformation η_ϵ of the underlying fibre bundle, namely,

$$\varphi_\epsilon = \eta_\epsilon \circ \varphi = \eta_\epsilon(\varphi) \quad (10.27)$$

such that the variational vector field $V : \mathcal{X} \rightarrow T\mathcal{Y}$ is defined as

$$V = \left. \frac{d}{d\epsilon} (\eta_\epsilon \circ \varphi) \right|_{\epsilon=0} = \left. \frac{d\eta_\epsilon}{d\epsilon}(\varphi) \right|_{\epsilon=0}, \quad (10.28)$$

or explicitly

$$V : x \mapsto \left((x, \varphi^a(x)), (0, V_\eta^a) \right) \quad (10.29)$$

where V_η is the generating vector field of the transformation η_ϵ with components

$$V_\eta^a = \left. \frac{d}{d\epsilon} \eta_\epsilon^a \right|_{\epsilon=0}, \quad (10.30)$$

η_ϵ^a being the y^a component of η_ϵ . For the moment, we are considering only vertical transformations as that is sufficient for the derivation of the Euler-Lagrange equations, but the Euler-Lagrange equations are also obtained for general variations, not necessarily of the form $\eta_\epsilon \circ \varphi$.

The flow map η_ϵ can be interpreted as dragging the path φ along V_η through the configuration space. From now on we drop the η index on the field components of the generating vector field. As we do not consider transformations in the coordinates this is no origin of confusion. The jet prolongation of V to $J^1\mathcal{Y}$ is given by

$$j^1V = \left. \frac{d}{d\epsilon} j^1(\eta_\epsilon \circ \varphi) \right|_{\epsilon=0} \quad (10.31)$$

or in coordinates

$$j^1V : x \mapsto \left((x^\mu, \varphi^a(x), \varphi_\nu^a(x)), (0, V^a, V_\nu^a + V_b^a \varphi_\nu^b) \right). \quad (10.32)$$

With this and

$$j^1\varphi_\epsilon = j^1(\eta_\epsilon \circ \varphi) = j^1\eta_\epsilon \circ j^1\varphi \quad (10.33)$$

such that

$$(j^1\varphi_\epsilon)^*\mathcal{L} = (j^1\varphi)^*(j^1\eta_\epsilon)^*\mathcal{L} \quad (10.34)$$

the action principle (10.26) can be rewritten as

$$\left. \frac{d}{d\epsilon} \mathcal{A}[\varphi_\epsilon] \right|_{\epsilon=0} = \frac{d}{d\epsilon} \left[\int_{\mathcal{X}} (j^1\varphi)^*(j^1\eta_\epsilon)^*\mathcal{L} \right]_{\epsilon=0} = 0. \quad (10.35)$$

With the dynamical definition of the Lie derivative (??),

$$\mathfrak{L}_{j^1V}\mathcal{L} = \left. \frac{d}{d\epsilon} [(j^1\eta_\epsilon)^*\mathcal{L}] \right|_{\epsilon=0}, \quad \text{and} \quad d\mathcal{A} \cdot V = \left. \frac{d}{d\epsilon} \mathcal{A}[\varphi_\epsilon] \right|_{\epsilon=0}, \quad (10.36)$$

(10.35) becomes a beautiful, general, geometric formulation of Hamilton's action principle

$$d\mathcal{A}[\varphi] \cdot V = \int_{\mathcal{X}} (j^1\varphi)^*(\mathfrak{L}_{j^1V}\mathcal{L}) = 0. \quad (10.37)$$

This form of the action principle has several advantages. First and most importantly, this equation is the very same for particles as well as for fields. Second, it makes explicit the use of the jet prolongation of the trajectory φ to $j^1\varphi$ and the variational vector field V to j^1V , whereas in the tangent bundle formulation, the tangent lift of φ and V is not explicit in the notation.

Last but not least, it is not too difficult to generalise from variations in the configuration space to variations in the full jet space. Thereby not only considering vertical variations, but general variations that might have both horizontal and vertical components.

Coming back to the derivation of the Euler-Lagrange equations, Cartan's magic formula

$$\mathfrak{L}_{j^1V}\mathcal{L} = i_{j^1V}d\mathcal{L} + d(i_{j^1V}\mathcal{L}) \quad (10.38)$$

needs to be employed to give

$$d\mathcal{A}[\varphi] \cdot V = \int_{\mathcal{X}} (j^1\varphi)^*(i_{j^1V}d\mathcal{L}) + \int_{\mathcal{X}} d((j^1\varphi)^*(i_{j^1V}\mathcal{L})) = 0 \quad (10.39)$$

where in the second integral we used that the pullback and the exterior derivative commute. The second integral vanishes due to Stokes' theorem and the assumption that the variations of φ vanish at the boundary $\partial\mathcal{X}$. Therefore, what is left is just

$$d\mathcal{A}[\varphi] \cdot V = \int_{\mathcal{X}} (j^1\varphi)^*(i_{j^1V}d\mathcal{L}) = 0. \quad (10.40)$$

This expression will be the basis for deriving the actual Euler-Lagrange equations in the jet bundle framework for both, particle mechanics and field theory, below.

Classical Mechanics on Jet Bundles

In classical mechanics, the base manifold is just time, $\mathcal{X} = \mathbb{R}$, with coordinates t . \mathcal{Y} is a fibre bundle over time, with the fibres \mathcal{Y}_t corresponding to the configuration space \mathcal{Q} , elements labelled by q and coordinates (t, q) , i.e., time and the generalised coordinates. The fibres $J^1_{(t,q)}\mathcal{Y}$ of the

first jet bundle $J^1\mathcal{Y}$ contain the time derivatives of all sections $c : \mathcal{X} \rightarrow \mathcal{Y}$. Its coordinates are (t, q, v) . The jet prolongation is given in coordinates by

$$j^1c : (t, c) \mapsto (t, c, \dot{c}). \quad (10.41)$$

Observe that $J^1\mathcal{Y}$ can be identified with (is isomorphic to) $\mathbb{R} \times T\mathcal{Q}$, sections of \mathcal{Y} correspond to trajectories $q(t)$ in \mathcal{Q} , sections of $J^1\mathcal{Y}$ to trajectories $(q(t), v(t))$ in $T\mathcal{Q}$, and that the jet prolongation is analogous to the tangent lift, such that holonomic sections j^1c of $J^1\mathcal{Y}$ are solutions $(q(t), \dot{q}(t))$ of the Euler-Lagrange equations. In classical mechanics the volume form is just $\omega = dt$. This implies that the Lagrangian is a function

$$L : J^1\mathcal{Y} \rightarrow \mathbb{R}. \quad (10.42)$$

The coordinate expression of \mathcal{L} is

$$\mathcal{L} = L(q, v) dt, \quad (10.43)$$

where we are considering a time-independent Lagrangian L . Starting from (10.40), compute the exterior derivative, contract with j^1V and do the usual integration by parts

$$d\mathcal{A}[c] \cdot V = \int_{\mathcal{X}} \left[\frac{\partial L}{\partial q}(j^1c) \cdot V + \frac{\partial L}{\partial v}(j^1c) \cdot \dot{V} \right] dt = \int_{\mathcal{X}} \left[\frac{\partial L}{\partial q}(j^1c) - \frac{d}{dt} \frac{\partial L}{\partial v}(j^1c) \right] \cdot V dt = 0. \quad (10.44)$$

The usual arguments then again yield the Euler-Lagrange equations

$$\frac{\partial L}{\partial q}(j^1c) - \frac{d}{dt} \frac{\partial L}{\partial v}(j^1c) = 0. \quad (10.45)$$

Note that in the jet bundle framework, the case of an explicit time dependency of the Lagrangian is automatically included.

Field Theory on Jet Bundles

In field theory, the base manifold \mathcal{X} is usually identified with spacetime. Its points are denoted x and its coordinates are (t, x, y, z) abbreviated as x^ν . \mathcal{Y} is thus a fibre bundle over spacetime with coordinates (x^ν, y^a) , where y^a are the different fields or field components of the theory, and the first jet bundle $J^1\mathcal{Y}$ has coordinates (x^ν, y^a, v_ν^a) . Hence, the Lagrangian density is a function $\mathcal{L}(x^\nu, y^a, v_\nu^a)$.

Considering a field theory of a (possibly vector valued) field $\varphi(x) : \mathcal{X} \rightarrow \mathcal{Y}$, defined over spacetime, one can directly start from the action principle as formulated in equation (10.37)

$$d\mathcal{A}[\varphi] \cdot V = \int_{\mathcal{X}} (j^1\varphi)^*(\mathfrak{L}_{j^1V}\mathcal{L}) = 0, \quad (10.46)$$

as all considerations that lead to this equation were completely general. All the hard work of section 10.1 is paying off now. The coordinate expressions of φ and V and their jet prolongations $j^1\varphi$ and j^1V are

$$\varphi : x \mapsto (x^\mu, \varphi^a), \quad j^1\varphi : x \mapsto (x^\mu, \varphi^a, \varphi_\mu^a), \quad (10.47a)$$

$$V : x \mapsto ((x^\mu, \varphi^a), (0, V^a)), \quad j^1V : x \mapsto ((x^\mu, \varphi^a, \varphi_\mu^a), (0, V^a, V_\mu^a)). \quad (10.47b)$$

Inserting this into (10.46) and making the exterior derivative, the contraction and the pullback explicit gives

$$d\mathcal{A}[\varphi] \cdot V = \int_{\mathcal{X}} \left[\frac{\partial L}{\partial y^a}(j^1\varphi) V^a + \frac{\partial L}{\partial v_\nu^a}(j^1\varphi) V_\nu^a \right] \omega \quad (10.48)$$

$$= \int_{\mathcal{X}} \left[\frac{\partial L}{\partial y^a}(j^1\varphi) - \frac{\partial}{\partial x^\nu} \frac{\partial L}{\partial v_\nu^a}(j^1\varphi) \right] V^a \omega \quad (10.49)$$

which leads to the Euler-Lagrange field equations,

$$\frac{\partial L}{\partial y^a}(j^1\varphi) - \frac{\partial}{\partial x^\nu} \frac{\partial L}{\partial v_\nu^a}(j^1\varphi) = 0, \quad (10.50)$$

that is the dynamical equations for a theory of a field φ on spacetime.

10.2 Variational Route to the Cartan Form

In this section we want to describe a variational derivation of the Cartan form, one of the two fundamental geometric structures of classical mechanics and classical field theories (the other one being the multisymplectic form, covered in the next section).

In most treatments, the Cartan form and the multisymplectic form are constructed by using the Legendre transformation to pull back the canonical forms from the Hamiltonian side (cotangent bundle) to the Lagrangian side (tangent bundle). However, it has been shown by Marsden, Patrick, and Shkoller [53] that the Cartan form arises naturally in the boundary term of the variation of the action in Hamilton's action principle, thus allowing to obtain these structures while staying on the Lagrangian side, entirely. The advantage of this approach is the possibility of a geometric treatment of theories for which a Hamiltonian cannot be defined.

After quickly reviewing the derivation of the Cartan one-form in the tangent bundle setting, which is restricted to autonomous systems of classical mechanics⁴, we will generalise the derivation to jet bundles and obtain an expression of the Cartan form that is valid for autonomous as well as non-autonomous systems of classical mechanics and also field theories.

Lagrangian One- and Two-Form

Besides leading to the equations of motion, the variational principle provides a direct and natural way to derive the fundamental geometric structures of classical mechanics⁵. For this derivation, the boundary conditions $\delta q(t_1) = \delta q(t_2) = 0$ are removed, while the time interval is kept fixed. Thus the variational principle reads

$$d\mathcal{A}[q(t)] \cdot \delta q(t) = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial v} \right] \cdot \delta q dt + \left[\frac{\partial L}{\partial v} \cdot \delta q \right]_{t_1}^{t_2} \quad (10.51)$$

⁴It is possible to derive the Cartan one-form for non-autonomous systems of classical mechanics in the tangent bundle framework (see Marsden and West [56], section 4.2), but it is not much clearer than the more general derivation on jet bundles.

⁵The following derivation follows along the lines of Marsden, Patrick, and Shkoller [53], section 2, and Marsden and Ratiu [54], section 8.2.

where the variations δq do not vanish at the boundary point, so that the last term on the right hand side does not vanish. This last term corresponds to a linear pairing of the function $\partial L/\partial v$, which is a function of (q, \dot{q}) , with the tangent vector δq . This term can be regarded as a one-form on $T\mathcal{Q}$ ⁶, referred to as the *Lagrangian one-form* or *Cartan one-form*,

$$\Theta_L = \frac{\partial L}{\partial v} dq. \quad (10.52)$$

This means that the Lagrangian one-form Θ_L is the boundary term of the functional derivative of the action, if the boundary is varied. The negative of the exterior derivative of the Lagrangian one-form gives the *Lagrangian two-form*, also referred to as the *symplectic two-form*

$$\Omega_L \equiv -d\Theta_L, \quad (10.53)$$

given in coordinates by

$$\Omega_L = \frac{\partial^2 L}{\partial q^i \partial v^j} dq^i \wedge dq^j + \frac{\partial^2 L}{\partial v^i \partial v^j} dv^i \wedge dq^j. \quad (10.54)$$

For details on the connection between the Lagrangian one-form Θ_L on $T\mathcal{Q}$ and the canonical one-form Θ on $T^*\mathcal{Q}$ as well as between the Lagrangian two-form Ω_L on $T\mathcal{Q}$ and the canonical symplectic two-form Ω on $T^*\mathcal{Q}$ the reader is referred to Marsden and Ratiu [54].

Cartan Form and Multisymplectic Form

To derive the Cartan form in a general setting that applies to classical mechanics as well as to field theories, the action principle on the jet bundle has to be generalised a bit further⁷. Before, only vertical variations of the action were considered, thereby implicitly restricting the treatment to Lagrangians, that are not explicitly time dependent in the case of particles, or do not explicitly depend on the coordinates in the case of fields, respectively. But in order to obtain the correct Cartan form in the general case also horizontal variations need to be considered. Whereas the Euler-Lagrange equations obtained by considering vertical or arbitrary variations are the same, the Cartan form is missing one term if only vertical variations are accounted for.

Allowing also for horizontal variations brings some complications. A transformation η acting on a section $\varphi : \mathcal{U}_{\mathcal{X}} \rightarrow \mathcal{Y}$, defined over a bounded domain $\mathcal{U}_{\mathcal{X}} \subset \mathcal{X}$,

$$\eta : (x, \varphi(x)) \mapsto (\eta_{\mathcal{X}}(x), \eta_{\mathcal{Y}}(x, \varphi(x))) \quad (10.55)$$

changes not only the section φ to $\eta \circ \varphi$ but also the base space from $\mathcal{U}_{\mathcal{X}}$ to $\eta_{\mathcal{X}}(\mathcal{U}_{\mathcal{X}})$. We explain now how to get around this issue.

Consider a smooth manifold \mathcal{U} with smooth closed boundary $\partial\mathcal{U}$. \mathcal{U} shall be a parametrisation of the space $\mathcal{U}_{\mathcal{X}} \subset \mathcal{X}$ on which the physical sections are defined. This is similar to the tangent bundle case, where a space of curves $\mathcal{C}(\mathcal{Q})$ was defined, such that elements of $\mathcal{C}(\mathcal{Q})$ correspond to

⁶One could be tempted to regard $\partial L/\partial \dot{q}$ as a one-form on \mathcal{Q} as it only has a component in dq . The same way δq could be regarded as a tangent vector on \mathcal{Q} . However, $\partial L/\partial \dot{q}$ is a function of (q, \dot{q}) and therefore clearly a function on $T\mathcal{Q}$. δq can also be replaced with a more general vector $\delta \hat{q} \in T(T\mathcal{Q})$ that has non-vanishing components $(\delta q, \delta v)$.

⁷The following derivation follows along the lines of Marsden, Patrick, and Shkoller [53, 57], Kouranbaeva and Shkoller [45], Kouranbaeva [44], chapter 4, and West [78], chapter 5.

parametrisations of the physical trajectories. Thus, in total analogy we define the set of smooth maps

$$\mathcal{C}(\mathcal{Y}) = \{\phi : \mathcal{U} \rightarrow \mathcal{Y} \mid \pi_{\mathcal{X}\mathcal{Y}} \circ \phi : \mathcal{U} \rightarrow \mathcal{X} \text{ is an embedding}\} \quad (10.56)$$

in coordinates

$$\phi : u \mapsto (x^\mu(u), \phi^a(u)) \quad \text{with} \quad x(u) \text{ an embedding,} \quad (10.57)$$

and $\phi^a(u)$ are the fibre coordinates of $\phi(u)$. Points in \mathcal{X} and \mathcal{U} are denoted x and u , respectively, and their coordinates are denoted x^μ and u^μ , respectively. For each $\phi \in \mathcal{C}(\mathcal{Y})$ define

$$\phi_{\mathcal{X}} \equiv \pi_{\mathcal{X}\mathcal{Y}} \circ \phi \quad \text{and} \quad \mathcal{U}_{\mathcal{X}} \equiv \pi_{\mathcal{X}\mathcal{Y}} \circ \phi(\mathcal{U}) \quad \text{such that} \quad \phi_{\mathcal{X}} : \mathcal{U} \rightarrow \mathcal{U}_{\mathcal{X}} \quad (10.58)$$

in coordinates

$$\phi_{\mathcal{X}} : u \mapsto x^\mu(u). \quad (10.59)$$

Since $\phi_{\mathcal{X}}$ is assumed to be an embedding, $\mathcal{U}_{\mathcal{X}}$ is a submanifold of \mathcal{X} that has a smooth closed boundary, just like \mathcal{U} . It is the physical space on which the fields and trajectories, i.e., the physical sections, are defined. Closed boundaries are necessary as the term we are interested in of the variational principle, the one that yields the Cartan form, is the boundary term that arises from the integration by parts.

The map $\phi_{\mathcal{X}}$ is a diffeomorphism between \mathcal{U} and $\mathcal{U}_{\mathcal{X}}$. It maps between the physical space and its parametrisation, such that the composition

$$\varphi = \phi \circ \phi_{\mathcal{X}}^{-1} \quad (10.60)$$

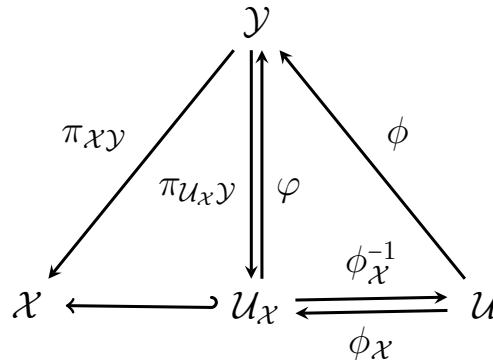
corresponds to a parametrisation of the sections that are physical fields or trajectories. These physical sections, defined on $\mathcal{U}_{\mathcal{X}}$, can be seen as sections of the fibre bundle represented by $\pi_{\mathcal{U}_{\mathcal{X}}, \mathcal{Y}}$. These are maps

$$\varphi : \mathcal{U}_{\mathcal{X}} \rightarrow \mathcal{Y} \quad \text{with} \quad \pi_{\mathcal{U}_{\mathcal{X}}, \mathcal{Y}} \circ \varphi = \pi_{\mathcal{X}\mathcal{Y}} \circ \varphi = \text{id} \quad (10.61)$$

in coordinates

$$\varphi : x \mapsto (x^\mu, \varphi^a(x)). \quad (10.62)$$

The fields that are varied in the action principle are the ϕ . Horizontal variations of the φ would change the base space $\mathcal{U}_{\mathcal{X}}$ on which the fields are defined. However, a transformation $\mathcal{Y} \rightarrow \mathcal{Y}$ acts naturally on the space \mathcal{C} , mapping \mathcal{C} into itself, even though $\mathcal{U}_{\mathcal{X}}$ is not mapped into itself.



To clarify some of the previous statements, consider the analogous derivation on tangent bundles. We defined $\mathcal{C}(\mathcal{Q})$ as the space of trajectories that connect two points in \mathcal{Q} . These trajectories $c \in \mathcal{C}(\mathcal{Q})$ were considered as maps

$$c : \mathcal{I} \rightarrow \mathcal{Q} \quad \text{with} \quad \mathcal{I} \subset \mathbb{R} \text{ smooth and bounded.} \quad (10.63)$$

In the jet bundle framework they correspond to elements of $\mathcal{C}(\mathcal{Y})$

$$c : \mathcal{U} \rightarrow \mathcal{Y}. \quad (10.64)$$

In the general case, the parameter space \mathcal{U} does not have just one dimension but as many as the base space \mathcal{X} . So the correspondence of the previous and the current notation is

$$\mathcal{I} \leftrightarrow \mathcal{U}, \quad \mathcal{Q} \leftrightarrow \mathcal{Y}, \quad \mathcal{C}(\mathcal{Q}) \leftrightarrow \mathcal{C}(\mathcal{Y}), \quad c \leftrightarrow \phi, \quad q \leftrightarrow \varphi.$$

Going back to the general theory, the tangent space to \mathcal{C} at a point ϕ is the set $T_\phi \mathcal{C}$ defined as

$$T_\phi \mathcal{C}(\mathcal{Y}) = \{V : \mathcal{U} \rightarrow T\mathcal{Y} \mid \pi_{\mathcal{Y}, T\mathcal{Y}} \circ V = \phi\}. \quad (10.65)$$

The elements V of $T_\phi \mathcal{C}$ are called variations of the sections ϕ and have coordinate expressions

$$V : u \mapsto \left((x^\mu(u), \varphi^a(u)), (V^\mu(u), V^a(u)) \right), \quad (10.66)$$

where the V^μ correspond to horizontal variations and the V^a to vertical variations. To each vector field V on $T_\phi \mathcal{C}$ belongs a vector field $V_\mathcal{X}$ on \mathcal{X} , given by projection

$$V_\mathcal{X} \equiv T\pi_{\mathcal{X}\mathcal{Y}} \circ V. \quad (10.67)$$

The projectors can be explicitly written as

$$\pi_{\mathcal{Y}, T\mathcal{Y}} : ((x^\mu, y^a), (V^\mu, V^a)) \mapsto (x^\mu, y^a), \quad (10.68)$$

$$T\pi_{\mathcal{X}\mathcal{Y}} : ((x^\mu, y^a), (V^\mu, V^a)) \mapsto (x^\mu, V^\mu), \quad (10.69)$$

such that $V_\mathcal{X}$ has the coordinate expression

$$V_\mathcal{X} : u \mapsto (x^\mu(u), V^\mu(u)). \quad (10.70)$$

The definition (10.65) of $T_\phi \mathcal{C}$ can also be seen by considering the variation of a path in $\mathcal{C}(\mathcal{Y})$,

$$\phi^\epsilon : u \mapsto (x^\mu(\epsilon, u), \phi^a(\epsilon, u)). \quad (10.71)$$

The derivatives of this expression and its projection to \mathcal{X} are

$$\left. \frac{d\phi^\epsilon}{d\epsilon} \right|_{\epsilon=0} = (V^\mu(u), V^a(u)), \quad (10.72)$$

which coincides with $V(u)$ in $T_{\phi(u)}\mathcal{Y}$, and

$$\left. \frac{d\phi_\mathcal{X}^\epsilon}{d\epsilon} \right|_{\epsilon=0} = \frac{d}{d\epsilon} \left[\pi_{\mathcal{X}\mathcal{Y}} \circ \phi^\epsilon \right] \Big|_{\epsilon=0} = T\pi_{\mathcal{X}\mathcal{Y}} V = V_\mathcal{X}. \quad (10.73)$$

To aid understanding some of these relations are depicted in the diagram below.

$$\begin{array}{ccccc}
 & & T\mathcal{Y} & \xrightarrow{T\pi_{\mathcal{X}\mathcal{Y}}} & T\mathcal{X} \\
 & \nearrow V & \downarrow \pi_{\mathcal{Y}, T\mathcal{Y}} & & \downarrow \pi_{\mathcal{X}, T\mathcal{X}} \\
 \mathcal{U} & \xrightarrow{\phi} & \mathcal{Y} & \xrightarrow{\pi_{\mathcal{X}\mathcal{Y}}} & \mathcal{X}
 \end{array}$$

Let us rephrase the action principle from the last section in this notation. The action functional

$$\mathcal{A} : \mathcal{C}(\mathcal{Y}) \rightarrow \mathbb{R} \quad (10.74)$$

is expressed as

$$\mathcal{A}[\phi] = \int_{\mathcal{U}_{\mathcal{X}}} (j^1\phi)^* \mathcal{L} = \int_{\mathcal{U}_{\mathcal{X}}} \mathcal{L}(j^1\phi) = \int_{\mathcal{U}_{\mathcal{X}}} \mathcal{L}(j^1(\phi \circ \phi_{\mathcal{X}}^{-1})). \quad (10.75)$$

As the action $\mathcal{A}[\phi]$ depends on ϕ only through φ , for any diffeomorphism $\gamma : \mathcal{U} \rightarrow \mathcal{U}$

$$\mathcal{A}[\phi \circ \gamma] = \mathcal{A}[\phi]. \quad (10.76)$$

As a consequence, the Euler-Lagrange equations only determine φ uniquely, not ϕ . However, as φ corresponds to the physical fields or trajectories, that is all we need. Hamilton's principle states that a section ϕ of $\mathcal{C}(\mathcal{Y})$ solves the Euler-Lagrange equations, iff the action is critical,

$$d\mathcal{A}[\phi] \cdot V = 0, \quad (10.77)$$

for all variations $V \in T_{\phi}\mathcal{C}(\mathcal{Y})$ which are zero on the boundary $\partial\mathcal{U}$ of \mathcal{U} . To derive the Cartan form, the last restriction has to be removed. The above expression corresponds to

$$d\mathcal{A}[\phi] \cdot V = \left. \frac{d}{d\epsilon} \mathcal{A}[\phi^{\epsilon}] \right|_{\epsilon=0} = 0. \quad (10.78)$$

A variation ϕ^{ϵ} of a section ϕ is induced by a transformation $\eta_{\mathcal{Y}}^{\epsilon}$ on the configuration space

$$\eta_{\mathcal{Y}}^{\epsilon} : \mathcal{Y} \rightarrow \mathcal{Y} \quad \text{with} \quad \eta_{\mathcal{Y}}^0 = \text{id} \quad (10.79)$$

through

$$\phi^{\epsilon} = \eta_{\mathcal{Y}}^{\epsilon} \circ \phi. \quad (10.80)$$

We impose the condition that $\eta_{\mathcal{Y}}^{\epsilon}$ covers a diffeomorphism

$$\eta_{\mathcal{X}}^{\epsilon} : \mathcal{X} \rightarrow \mathcal{X}. \quad (10.81)$$

In coordinates

$$\eta_{\mathcal{Y}}^{\epsilon} : (x, y) \mapsto (\eta_{\mathcal{X}}^{\mu}(x), \eta_{\mathcal{Y}}^a(x, y)). \quad (10.82)$$

The diffeomorphism on the base space \mathcal{X} is obtained through the projection

$$\eta_{\mathcal{X}}^{\epsilon} = \pi_{\mathcal{X}\mathcal{Y}} \circ \eta_{\mathcal{Y}}^{\epsilon}. \quad (10.83)$$

The following diagram should help clarify these relations.

$$\begin{array}{ccc}
 \mathcal{Y} & \xrightarrow{\eta_{\mathcal{Y}}^{\epsilon}} & \mathcal{Y} \\
 \uparrow \varphi & & \uparrow \varphi^{\epsilon} \\
 \mathcal{U}_{\mathcal{X}} & \xrightarrow{\eta_{\mathcal{X}}^{\epsilon}} & \eta_{\mathcal{X}}^{\epsilon}(\mathcal{U}_{\mathcal{X}})
 \end{array}$$

We see now why it is necessary to introduce a parameter space \mathcal{U} . A physical section $\varphi = \phi \circ \phi_{\mathcal{X}}^{-1}$ is a section of $\pi_{\mathcal{U}_{\mathcal{X}}, \mathcal{Y}}$. But the transformation $\eta_{\mathcal{Y}}^{\epsilon} \circ \phi$ induces a section $\varphi^{\epsilon} = \eta_{\mathcal{Y}}^{\epsilon} \circ (\phi \circ \phi_{\mathcal{X}}^{-1}) \circ (\eta_{\mathcal{X}}^{\epsilon})^{-1}$ of $\pi_{\eta_{\mathcal{X}}^{\epsilon}(\mathcal{U}_{\mathcal{X}}), \mathcal{Y}}$, i.e., the base space itself changes under the transformation. This becomes more evident by looking at the coordinate expressions

$$\phi : u \mapsto (x^{\mu}(u), \phi^a(u)), \quad \phi^{\epsilon} : u \mapsto (\eta_{\mathcal{X}}^{\mu}(x(u)), \eta_{\mathcal{Y}}^a(x(u), \phi(u))), \quad (10.84a)$$

$$\varphi : x \mapsto (x^{\mu}, \phi^a(x)), \quad \varphi^{\epsilon} : \tilde{x} \mapsto (\tilde{x}^{\mu}, \eta_{\mathcal{Y}}^a(x, \varphi(x))), \quad (10.84b)$$

where $\tilde{x} \in \eta_{\mathcal{X}}^{\epsilon}(\mathcal{U}_{\mathcal{X}})$ and $x = (\eta_{\mathcal{X}}^{\epsilon})^{-1}(\tilde{x}) \in \mathcal{U}_{\mathcal{X}}$. If we consider not variations of the physical sections $\varphi : \mathcal{U}_{\mathcal{X}} \rightarrow \mathcal{Y}$ but variations of the sections $\phi : \mathcal{U} \rightarrow \mathcal{Y}$, the point u in the base space \mathcal{U} stays fixed. Applying the transformation (10.79) to the action (10.75), the variation (10.78) becomes

$$d\mathcal{A}[\phi] \cdot V = \left. \frac{d}{d\epsilon} \mathcal{A}[\eta_{\mathcal{Y}}^{\epsilon} \circ \phi] \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} \int_{\eta_{\mathcal{X}}^{\epsilon}(\mathcal{U}_{\mathcal{X}})} \mathcal{L}(j^1 \varphi^{\epsilon}) \right|_{\epsilon=0} = \int_{\mathcal{U}_{\mathcal{X}}} \left. \frac{d}{d\epsilon} (\eta_{\mathcal{X}}^{\epsilon})^* \mathcal{L}(j^1 \varphi^{\epsilon}) \right|_{\epsilon=0}. \quad (10.85)$$

Application of the chain rule yields

$$d\mathcal{A}[\phi] \cdot V = \int_{\mathcal{U}_{\mathcal{X}}} \left. \frac{d}{d\epsilon} \left[(\eta_{\mathcal{X}}^{\epsilon})^* \mathcal{L}(j^1 \varphi^0) \right] \right|_{\epsilon=0} + \int_{\mathcal{U}_{\mathcal{X}}} \left. \frac{d}{d\epsilon} \left[(\eta_{\mathcal{X}}^0)^* \mathcal{L}(j^1 \varphi^{\epsilon}) \right] \right|_{\epsilon=0}. \quad (10.86)$$

In the first integral, apply the dynamical definition of the Lie derivative as before in (10.36), and in the second integral realise that $\eta_{\mathcal{X}}^0$ is just the identity

$$d\mathcal{A}[\phi] \cdot V = \int_{\mathcal{U}_{\mathcal{X}}} \mathbf{L}_{V_{\mathcal{X}}} \mathcal{L}(j^1 \varphi) + \int_{\mathcal{U}_{\mathcal{X}}} \left. \frac{d}{d\epsilon} \left[\mathcal{L}(j^1 \varphi^{\epsilon}) \right] \right|_{\epsilon=0}. \quad (10.87)$$

Use Cartan's magic formula in the first integral, and rewrite the second integral by making use of the identity

$$\left. \frac{d}{d\epsilon} \left[\mathcal{L}(j^1 \varphi^{\epsilon}) \right] \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} \left[L(j^1 \varphi^{\epsilon}) \right] \right|_{\epsilon=0} \omega = \left(\mathbf{z}_{j^1 V_{\varphi}} dL(j^1 \varphi) \right) \omega, \quad (10.88)$$

such that

$$d\mathcal{A}[\phi] \cdot V = \int_{\mathcal{U}_{\mathcal{X}}} \mathbf{z}_{V_{\mathcal{X}}} d\mathcal{L}(j^1 \varphi) + \int_{\mathcal{U}_{\mathcal{X}}} d(\mathbf{z}_{V_{\mathcal{X}}} \mathcal{L}(j^1 \varphi)) + \int_{\mathcal{U}_{\mathcal{X}}} (\mathbf{z}_{j^1 V_{\varphi}} dL(j^1 \varphi)) \omega. \quad (10.89)$$

The first integral vanishes as $\mathcal{L} = L\omega$ and therefore

$$d\mathcal{L}(j^1\varphi) = dL(j^1\varphi) \wedge \omega + L(j^1\varphi) d\omega = L_\mu(j^1\varphi) dx^\mu \wedge \omega + L(j^1\varphi) d\omega = 0, \quad (10.90)$$

but $\omega = dx^1 \wedge \dots \wedge dx^n$ is a form of maximum order on the base space, such that $d\omega = 0$ and $dx^\mu \wedge \omega = 0$ for all μ . By Stokes' theorem, the second integral can be transformed into a surface integral, with the result that

$$d\mathcal{A}[\phi] \cdot V = \int_{\partial\mathcal{U}_\mathcal{X}} \mathbf{i}_{V_\mathcal{X}} \mathcal{L}(j^1\varphi) + \int_{\mathcal{U}_\mathcal{X}} \left(\mathbf{i}_{j^1 V_\varphi} dL(j^1\varphi) \right) \omega. \quad (10.91)$$

Now we have to compute the vector field V_φ corresponding to the transformation of the physical section φ

$$V_\varphi = \left. \frac{d}{d\epsilon} \varphi^\epsilon \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} \left[\eta_Y^\epsilon \circ (\phi \circ \phi_X^{-1}) \circ (\eta_X^\epsilon)^{-1} \right] \right|_{\epsilon=0}, \quad (10.92)$$

and its jet prolongation $j^1 V_\varphi$. Applying the chain rule, we get

$$V_\varphi = \left. \frac{d}{d\epsilon} \left[\eta_Y^\epsilon \circ (\phi \circ \phi_X^{-1}) \circ (\eta_X^0)^{-1} \right] \right|_{\epsilon=0} + \left. \frac{d}{d\epsilon} \left[\eta_Y^0 \circ (\phi \circ \phi_X^{-1}) \circ (\eta_X^\epsilon)^{-1} \right] \right|_{\epsilon=0}. \quad (10.93)$$

In the first term we use (10.72) and in the second term we use the fact that $d/d\epsilon (\eta_X^\epsilon)^{-1}|_{\epsilon=0} = -V_X^8$, such that

$$V_\varphi = V \circ \phi_X^{-1} - T(\phi \circ \phi_X^{-1}) \circ V_X. \quad (10.94)$$

The tangent lift of the vector field V_X is simply

$$T(\phi \circ \phi_X^{-1}) \circ V_X = \left((x^\nu, \varphi^a(x)), (V^\nu, \varphi_\mu^a V^\mu) \right) \quad (10.95)$$

such that

$$V_\varphi = (0, \delta\varphi^a) = (0, V^a - \varphi_\mu^a V^\mu). \quad (10.96)$$

⁸This can be seen by the group property of the transformation

$$\eta_X^{-\epsilon} = (\eta_X^\epsilon)^{-1} \quad \rightarrow \quad -V_X = \left. \frac{d}{d\epsilon} \eta_X^{-\epsilon} \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} (\eta_X^\epsilon)^{-1} \right|_{\epsilon=0}$$

or by a simple calculation as follows

$$\eta_X^\epsilon \circ (\eta_X^\epsilon)^{-1} = \eta_X(\epsilon, \eta_X^{-1}(\epsilon, x)) = \text{id}$$

such that

$$\left. \frac{d}{d\epsilon} \left[\eta_X^\epsilon \circ (\eta_X^\epsilon)^{-1} \right] \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} \left[\eta_X^\epsilon \circ (\eta_X^0)^{-1} \right] \right|_{\epsilon=0} + \left. \frac{d}{d\epsilon} \left[\eta_X^0 \circ (\eta_X^\epsilon)^{-1} \right] \right|_{\epsilon=0} = 0.$$

$\eta_X^0 = \text{id}$ and $(\eta_X^0)^{-1} = \text{id}^{-1} = \text{id}$ as well, such that

$$\left. \frac{d}{d\epsilon} \left[\eta_X^\epsilon \circ (\eta_X^\epsilon)^{-1} \right] \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} \left[\eta_X^\epsilon \right] \right|_{\epsilon=0} + T \text{id} \circ \left. \frac{d}{d\epsilon} \left[(\eta_X^\epsilon)^{-1} \right] \right|_{\epsilon=0} = V_X + \left. \frac{d}{d\epsilon} (\eta_X^\epsilon)^{-1} \right|_{\epsilon=0} = 0,$$

where the tangent lift of the identity is the identity on the tangent space.

This is just the vertical component of the vector field V from (10.66)⁹. The jet prolongation of V_φ along $j^1\varphi$ is

$$j^1V_\varphi = (0, \delta\varphi^a, \delta\varphi_\nu^a) = \left(0, V^a - \varphi_\mu^a V^\mu, \partial_\nu(V^a - \varphi_\mu^a V^\mu)\right). \quad (10.97)$$

With that we compute the action (10.91) as

$$d\mathcal{A}[\phi] \cdot V = \int_{\mathcal{U}_\mathcal{X}} \left[\frac{\partial L}{\partial y^a}(j^1\varphi) \delta\varphi^a + \frac{\partial L}{\partial v_\mu^a}(j^1\varphi) \delta\varphi_\mu^a \right] \omega + \int_{\partial\mathcal{U}_\mathcal{X}} L(j^1\varphi) V^\mu \omega_\mu \quad (10.98)$$

where $\omega_\mu = \partial_\mu \lrcorner \omega$. Integrate by parts the second term of the first integral

$$\begin{aligned} d\mathcal{A}[\phi] \cdot V &= \int_{\mathcal{U}_\mathcal{X}} \left[\frac{\partial L}{\partial y^a}(j^1\varphi) - \frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial v_\mu^a}(j^1\varphi) \right) \right] \delta\varphi^a \omega \\ &\quad + \int_{\partial\mathcal{U}_\mathcal{X}} \left[L(j^1\varphi) V^\mu + \frac{\partial L}{\partial v_\mu^a}(j^1\varphi) V^a - \frac{\partial L}{\partial v_\mu^a}(j^1\varphi) \varphi_\nu^a V^\nu \right] \omega_\mu. \end{aligned} \quad (10.99)$$

To bring this expression into a coordinate-free form, consider a general vector field $W = (W^\nu, W^a, W_\nu^a)$. Its contraction with $dy^a \wedge \omega$ is given by

$$\mathfrak{z}_W(dy^a \wedge \omega) = W^a \omega - (-1)^{p^\nu} W^\nu dy^a \wedge \omega_\nu \quad (10.100)$$

where p^ν is the number of permutations in the computation of $\omega_\nu = \partial_\nu \lrcorner \omega$ (the additional minus results from the permutation with dy^a). The pullback of this relation with $j^1\varphi$ is

$$(j^1\varphi)^* \mathfrak{z}_W(dy^a \wedge \omega) = W^a(j^1\varphi) \omega - (-1)^{p^\nu} W^\nu \varphi_\nu^a dx^\nu \wedge \omega_\nu = (W^a(j^1\varphi) - W^\nu \varphi_\nu^a) \omega. \quad (10.101)$$

Applying this result to the variation of the action (10.99), we find

$$(j^1\varphi)^* \mathfrak{z}_{j^1V}(dy^a \wedge \omega) = \delta\varphi^a \omega. \quad (10.102)$$

Further, consider the expression

$$\mathfrak{z}_W(dy^a \wedge \omega_\nu) = W^a \omega_\nu - (-1)^{p^\mu} W^\mu dy^a \wedge \omega_{\nu\mu}. \quad (10.103)$$

With

$$dx^\sigma \wedge \omega_{\nu\mu} = \begin{cases} 0 & \sigma \neq \mu, \nu \\ \omega_\nu & \mu = \sigma \\ -\omega_\mu & \nu = \sigma \end{cases} \quad (10.104)$$

the pullback of (10.103) with $j^1\varphi$ is

$$\begin{aligned} (j^1\varphi)^* \mathfrak{z}_W(dy^a \wedge \omega_\mu) &= W^a \omega_\mu - (-1)^{p^\nu} W^\nu \varphi_\sigma^a dx^\sigma \wedge \omega_{\mu\nu} \\ &= W^a \omega_\mu - W^\nu \varphi_\nu^a \omega_\mu + \varphi_\mu^a W^\nu \omega_\mu. \end{aligned} \quad (10.105)$$

⁹Any vector $V \in T_\phi\mathcal{C}$ can be decomposed into a horizontal and a vertical component $V = V^h + V^v$, where $V^h = T\varphi \circ V_\mathcal{X}$ and $V^v = V - V^h$.

Applying this result to the variation of the action (10.99), we find

$$\begin{aligned} (j^1\varphi)^*\iota_V(dy^a \wedge \omega_\mu) &= V^a \omega_\mu - V^\sigma \varphi_\nu^a dx^\nu \wedge \omega_{\mu\sigma} = V^a \omega_\mu - V^\sigma \varphi_\nu^a (\omega_\mu \delta_\sigma^\nu - \omega_\sigma \delta_\mu^\nu) \\ &= V^a \omega_\mu - V^\nu \varphi_\nu^a \omega_\mu + V^\nu \varphi_\mu^a \omega_\nu. \end{aligned} \quad (10.106)$$

A final but simple computation shows

$$(j^1\varphi)^*\iota_{j^1V}\omega = V^\mu \omega_\mu. \quad (10.107)$$

Therefore, the variation of the action (10.99) can be written as

$$\begin{aligned} d\mathcal{A}[\phi] \cdot V &= \int_{\mathcal{U}_X} (j^1\varphi)^*\iota_{j^1V} \left[\frac{\partial L}{\partial y^a} - \frac{\partial}{\partial x^\mu} \frac{\partial L}{\partial v_\mu^a} \right] dy^a \wedge \omega \\ &\quad + \int_{\partial\mathcal{U}_X} (j^1\varphi)^*\iota_{j^1V} \left[\frac{\partial L}{\partial v_\mu^a} dy^a \wedge \omega_\mu + \left(L - \frac{\partial L}{\partial v_\mu^a} \varphi_\mu^a \right) \omega \right]. \end{aligned} \quad (10.108)$$

In the first integral we find the Euler-Lagrange equations as we derived them before by considering only vertical variations (10.50). The expression in square brackets in the second integral is the looked for Cartan form

$$\Theta_L = \frac{\partial L}{\partial v_\mu^a} dy^a \wedge \omega_\mu + \left(L - \frac{\partial L}{\partial v_\mu^a} \varphi_\mu^a \right) \omega. \quad (10.109)$$

In the case of particle mechanics, this is a one-form, otherwise it is a form of the order of the base manifold. The *symplectic form* is defined as the exterior derivative of the Cartan form

$$\Omega_L = -d\Theta_L = dy^a \wedge d\left(\frac{\partial L}{\partial v_\mu^a}\right) \wedge \omega_\mu - d\left(L - \frac{\partial L}{\partial v_\mu^a} \varphi_\mu^a\right) \wedge \omega. \quad (10.110)$$

Both, the Cartan and the symplectic form, are defined on the first jet bundle, i.e., $\Theta_L \in \Omega^1$ and $\Omega_L \in \Omega^2$. Using these expressions, the variation of the action (10.108) can be written as

$$d\mathcal{A}[\phi] \cdot V = \int_{\mathcal{U}_X} (j^1\varphi)^*(\iota_{j^1V}\Omega_L) + \int_{\partial\mathcal{U}_X} (j^1\varphi)^*(\iota_{j^1V}\Theta_L). \quad (10.111)$$

This will be the starting point to prove the preservation of the multisymplectic form along the Lagrangian flow in section (10.3). The expressions (10.109) and (10.110) are more general than the ones we derived previously, (10.52) and (10.53), in that they lift the restriction to a time-independent Lagrangian and describe field theories as well.

10.3 Preservation of the Multisymplectic Form

In this section we want to show that the multisymplectic form Ω_L from (10.110) is preserved under the Lagrangian flow, a generalisation of the results from the previous section. Therefore we recall equation (10.111) for the variation of the action, that is

$$d\mathcal{A}[\phi] \cdot V = \int_{\mathcal{U}_X} (j^1\varphi)^*(\iota_{j^1V}\Omega_L) + \int_{\partial\mathcal{U}_X} (j^1\varphi)^*(\iota_{j^1V}\Theta_L). \quad (10.112)$$

The action \mathcal{A} takes an extremum for $\phi \in \mathcal{C}(\mathcal{Y})$ if the first integral vanishes. The corresponding integrand vanishes not only for vector fields j^1V , corresponding to vertical transformations, but for general vector fields W on $J^1\mathcal{Y}$, that can be tangent to any $j^1\phi$. As a consequence, ϕ is an extremum of the action, if the variation of the action (10.112) vanishes for all vectors $W \in T(J^1\mathcal{Y})$. Such ϕ are solutions of the Euler-Lagrange equations (10.50).

We define \mathcal{C}_L to be the restriction of $\mathcal{C}(\mathcal{Y})$, defined in (10.56), to solutions of the Euler-Lagrange equations, i.e.,

$$\mathcal{C}_L = \{ \phi \in \mathcal{C}(\mathcal{Y}) \mid (j^1\phi)^*[W \lrcorner \Omega_L] = 0 \text{ for all } W \in T(J^1\mathcal{Y}) \}, \quad (10.113)$$

such that φ^a is an element of \mathcal{C}_L if

$$\frac{\partial L}{\partial y^a}(j^1\varphi) - \frac{\partial}{\partial x^\mu} \left(\frac{\partial L}{\partial v_\mu^a}(j^1\varphi) \right) = 0 \text{ in } \mathcal{U}_X. \quad (10.114)$$

A vector field $V \in T\mathcal{C}_L$ is called a first variation. Its flow maps solutions ϕ of the Euler-Lagrange equations to other solutions of the Euler-Lagrange equations, such that sections $\phi \in \mathcal{C}_L$ are integral curves of V .

If we restrict the variation of the action to \mathcal{C}_L , the first integral in (10.112) becomes zero. Computing the exterior derivative of (10.112) and restricting it to two first variations $V, W \in T\mathcal{C}_L$, gives

$$0 = d^2\mathcal{A}[\phi] \cdot V \cdot W = \int_{\partial\mathcal{U}_X} (j^1\varphi)^*(V \lrcorner W \lrcorner d\Theta_L). \quad (10.115)$$

This states that the multisymplectic form Ω_L is conserved in the so called Multisymplectic Form Formula,

$$\int_{\partial\mathcal{U}_X} (j^1\varphi)^*(V \lrcorner W \lrcorner \Omega_L) = 0. \quad (10.116)$$

A detailed proof of this expression is omitted but can be found in Marsden, Patrick, and Shkoller [53].

10.4 Noether Theorem

The Noether theorem [63, 43] states that each Lie point symmetry of a Lagrangian corresponds to a conservation law of the associated Euler-Lagrange equations.

We restrict our attention to conservation laws that are generated by vertical transformations of the configuration bundle Y , i.e., transformations which leave the base space X invariant. In the framework of formal Lagrangians addressed below, this is often sufficient to uncover interesting conservation laws (including conservation of momentum and energy). Our derivation of the Noether theorem is essentially based on reference [53].

A transformation is generated by a map $\sigma^\epsilon(x, y)$, that is

$$\varphi^\epsilon = \sigma^\epsilon \circ \varphi \quad \text{with} \quad \sigma^\epsilon|_{\epsilon=0} = \text{id} \quad \text{and} \quad V = \left. \frac{d\sigma^\epsilon}{d\epsilon} \right|_{\epsilon=0}, \quad (10.117)$$

but it is not required that σ^ϵ reduces to the identity at boundary points. In our analysis we will usually just prescribe the generating vector field V instead of the actual transformation σ^ϵ . In components, V can be written as

$$V(x, y) = \eta^a(x, y) \frac{\partial}{\partial y^a} \quad \text{with} \quad \eta^a(x, y) = \left. \frac{d}{d\epsilon} (\sigma^\epsilon)^a(x, y) \right|_{\epsilon=0}, \quad (10.118)$$

where $(\sigma^\epsilon)^a$ is the a -th component of the transformation map. Since Lagrangians are functions defined on J^1Y , we need to compute the first prolongation of the generating vector field. The prolongation of V is defined via the jet prolongation of the transformation map σ^ϵ ,

$$j^1V = \left. \frac{d}{d\epsilon} [j^1\sigma^\epsilon(x, y)] \right|_{\epsilon=0}, \quad (10.119)$$

and is given by

$$j^1V = \eta^a \frac{\partial}{\partial y^a} + \left(\frac{\partial \eta^a}{\partial x^\mu} + z_\mu^b \frac{\partial \eta^a}{\partial y^b} \right) \frac{\partial}{\partial z_\mu^a} = \eta^a \frac{\partial}{\partial y^a} + \eta_\mu^a \frac{\partial}{\partial z_\mu^a}. \quad (10.120)$$

A vertical transformation σ^ϵ is a symmetry transformation for the Lagrangian L if the invariance condition,

$$L(j^1(\sigma^\epsilon \circ \varphi)) = L(j^1\varphi), \quad (10.121)$$

is satisfied¹⁰. Taking the ϵ derivative of (10.121), we obtain an infinitesimal invariance condition,

$$\left. \frac{d}{d\epsilon} L(j^1(\sigma^\epsilon \circ \varphi)) \right|_{\epsilon=0} = 0, \quad (10.122)$$

which is equivalent to (10.121). Explicitly computing the ϵ derivative, we obtain

$$j^1V(L)(j^1\varphi) = \frac{\partial L}{\partial y^a}(j^1\varphi) \cdot \eta^a(\varphi) + \frac{\partial L}{\partial z_\mu^a}(j^1\varphi) \cdot \left[\frac{\partial \eta^a}{\partial x^\mu} + \frac{\partial \eta^a}{\partial y^b} \frac{\partial \varphi^b}{\partial x^\mu} \right] = 0. \quad (10.123)$$

If φ solves the Euler-Lagrange field equations, we can replace the first term on the right-hand side of (10.123) to obtain

$$\left[\frac{\partial}{\partial x^\mu} \frac{\partial L}{\partial z_\mu^a}(j^1\varphi) \right] \cdot \eta^a(\varphi) + \frac{\partial L}{\partial z_\mu^a}(j^1\varphi) \cdot \left[\frac{\partial \eta^a}{\partial x^\mu} + \frac{\partial \eta^a}{\partial y^b} \frac{\partial \varphi^b}{\partial x^\mu} \right] = 0. \quad (10.124)$$

This, at last, amounts to a total divergence,

$$\operatorname{div} [J(j^1\varphi)] = 0, \quad (10.125)$$

with the Noether current J given by

$$J^\mu(j^1\varphi) = \frac{\partial L}{\partial z_\mu^a}(j^1\varphi) \cdot \eta^a(\varphi). \quad (10.126)$$

The fact that the Noether current is divergence-free, expresses the conservation law satisfied by solutions φ of the Euler-Lagrange field equations. The flux of J through the boundary of any domain $\Omega \subseteq X$ is zero.

¹⁰Here, invariance of the Lagrangian suffices, but for general transformations, i.e., transformations that transform the base space in addition to the configuration space, invariance of the Lagrangian does not guarantee that φ^ϵ is a solution whenever φ is a solution. Invariance of solutions requires invariance of the action, and invariance of the action requires equivariance of the Lagrangian, which also takes the deformation of the integration domain X into account. For a detailed discussion see, e.g., Lew et al. [51], section 6.5.

Global Form of Conservation Laws

Let us consider an alternative point of view that is better suited for actual computations on the discrete level. If the Lagrangian is invariant under the vertical transformation (10.117), the action is also invariant under this transformation,

$$\left. \frac{d}{d\epsilon} \mathcal{A}[\sigma^\epsilon \circ \varphi] \right|_{\epsilon=0} = \int_X j^1 V(L)(j^1 \varphi) d^{n+1}x = 0. \quad (10.127)$$

Repeating the steps that lead from (10.123) to (10.125) this becomes

$$\left. \frac{d}{d\epsilon} \mathcal{A}[\sigma^\epsilon \circ \varphi] \right|_{\epsilon=0} = \int_X \frac{\partial}{\partial x^\mu} \left[\frac{\partial L}{\partial z_\mu^a} (j^1 \varphi) \cdot \eta^a(\varphi) \right] d^{n+1}x = 0. \quad (10.128)$$

With appropriate boundary conditions, one has

$$\int \frac{\partial}{\partial x^i} \left[\frac{\partial L}{\partial z_i^a} (j^1 \varphi) \cdot \eta^a(\varphi) \right] d^n x = 0, \quad (10.129)$$

and thus, integrating (10.128) for $x^0 = t \in [t_0, t_1]$,

$$\left. \frac{d}{d\epsilon} \mathcal{A}[\sigma^\epsilon \circ \varphi] \right|_{\epsilon=0} = \left[\int \frac{\partial L}{\partial z_t^a} (j^1 \varphi) \cdot \eta^a(\varphi) d^n x \right]_{t_0}^{t_1} = 0. \quad (10.130)$$

This is equivalent to integrating the divergence of the Noether current (10.125) over the spatial dimensions and using (10.129). Since t_0 and t_1 are arbitrary, this implies the conservation of

$$\mathcal{J} = \int \frac{\partial L}{\partial z_t^a} (j^1 \varphi) \cdot \eta^a(\varphi) d^n x = \int J^t(j^1 \varphi) d^n x, \quad (10.131)$$

which is called Noether charge.

Divergence Symmetries

Sometimes it is necessary to consider a slightly more general version of Noether's theorem [66]. The invariance condition (10.123) can be weakened to

$$j^1 V(L)(j^1 \varphi) = \operatorname{div} B(j^1 \varphi), \quad (10.132)$$

with B being a vector field over Y of the form $B = B^\mu(x, y) \partial / \partial x^\mu$, and $\operatorname{div} B$ is a scalar field defined over $J^1 Y$ given by

$$\operatorname{div} B(x, y, z) = \frac{\partial B^\mu(x, y)}{\partial x^\mu} + \frac{\partial B^\mu(x, y)}{\partial y^a} z_\mu^a. \quad (10.133)$$

This form of the invariance condition is tightly related to the gauge freedom of the Lagrangian. We can add any divergence to the Lagrangian without changing the equations of motion as

$$\mathcal{A}[\varphi] = \int_X L'(j^1 \varphi) d^{n+1}x = \int_X (L + \operatorname{div} H)(j^1 \varphi) d^{n+1}x = \int_X L(j^1 \varphi) d^{n+1}x, \quad (10.134)$$

assuming appropriate boundary conditions. Here, H is a vector field over Y of the form $H = H^\mu(x, y) \partial/\partial x^\mu$, $\text{div } H$ is defined as in (10.133), and

$$L'(x, y, z) = (L + \text{div } H)(x, y, z). \quad (10.135)$$

One can check that the Euler-Lagrange equations for L and L' are the same. Requiring the invariance condition (10.123) to be satisfied for L' ,

$$j^1 V(L')(j^1 \varphi) = j^1 V(L)(j^1 \varphi) + \text{div } \tilde{H}(j^1 \varphi) = 0, \quad \text{with} \quad \tilde{H} = V(H^\mu) \frac{\partial}{\partial x^\mu}, \quad (10.136)$$

we find the following relation between the vector fields B and H ,

$$B = -\tilde{H}. \quad (10.137)$$

In summary, if V is a divergence symmetry for L in the sense of (10.132) and there exists a vector field H satisfying (10.137), then V is a Lie-point symmetry (10.123) of the equivalent Lagrangian L' defined in (10.135). We can therefore apply the Noether theorem to L' , obtaining the Noether current

$$J'(j^1 \varphi) = J(j^1 \varphi) - B(\varphi), \quad (10.138)$$

with J' the conserved Noether current associated to the divergence symmetry (10.132) and J as defined in (10.126), which is not conserved in this case.

11 Variational Integrators for Partial Differential Equations

The derivation of the discrete field theory is a straight forward generalisation of the derivation for particle dynamics. The only difference is that the basic physical quantity is not the Lagrangian, defined on a one-dimensional “grid” of time, but the Lagrangian density, defined over a multidimensional grid of spacetime.

Again, the starting point is the discretisation of the action integral and the Lagrangian density. The discrete Lagrangian density approximates the spacetime integral of the continuous Lagrangian density over one cell of the spacetime grid, e.g. with one spatial dimension this is

$$L_d(\varphi_{i,n}, \varphi_{i+1,n}, \varphi_{i,n+1}, \varphi_{i+1,n+1}) \approx \int_{t_n}^{t_{n+1}} \int_{x_i}^{x_{i+1}} L(\varphi, \varphi_t, \varphi_x) dt dx, \quad (11.1)$$

with the corresponding action being a sum over the whole grid

$$\mathcal{A}_d = \sum_{n=0}^{N_t-1} \sum_{i=0}^{N_x-1} L_d(\varphi_{i,n}, \varphi_{i+1,n}, \varphi_{i,n+1}, \varphi_{i+1,n+1}). \quad (11.2)$$

To make manipulations more tractable, the discrete Lagrangian density is rewritten in a slightly more abstract way, namely in terms of cells rather than grid points. Let us consider a cell determined by its vertices $(\varphi^1, \varphi^2, \varphi^3, \varphi^4)$, like it is depicted in Fig. 11.1. For now, the horizontal axis shall be space, denoted by x , and the vertical axis shall be time, denoted by t .

Here, only a midpoint rule is considered, but the application of other quadrature rules is straight forward. The fields φ are thus approximated by

$$\varphi(t, x) \approx \frac{1}{4}(\varphi^1 + \varphi^2 + \varphi^3 + \varphi^4). \quad (11.3)$$

For the approximation of the derivatives, there are in principle two possibilities for each coordinate, e.g. an x derivative can be defined as $(\varphi^2 - \varphi^1)/h_x$ as well as $(\varphi^3 - \varphi^4)/h_x$. Again, a midpoint-like

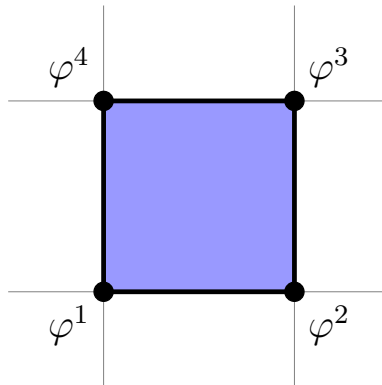


Fig. 11.1: Basic element of a two-dimensional spacetime grid.

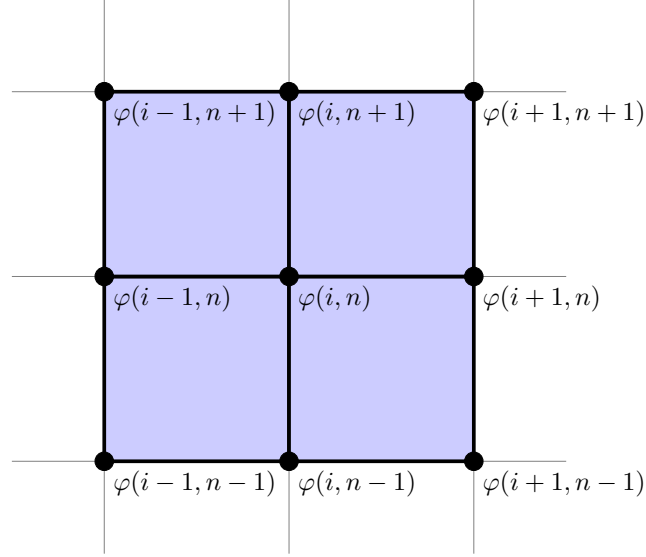


Fig. 11.2: Contributions of a specific grid point (i, n) to the variation of the discrete action.

averaging over the two possibilities is employed, such that

$$\varphi_t(t, x) \approx \frac{1}{2} \left(\frac{\varphi^4 - \varphi^1}{h_t} + \frac{\varphi^3 - \varphi^2}{h_t} \right), \quad \varphi_x(t, x) \approx \frac{1}{2} \left(\frac{\varphi^2 - \varphi^1}{h_x} + \frac{\varphi^3 - \varphi^4}{h_x} \right). \quad (11.4)$$

Applying this to (11.1), the resulting discrete Lagrangian density reads

$$L_d(\varphi^1, \varphi^2, \varphi^3, \varphi^4) \approx h_t h_x L \left(\frac{\varphi^1 + \varphi^2 + \varphi^3 + \varphi^4}{4}, \frac{\varphi^4 - \varphi^1}{2h_t} + \frac{\varphi^3 - \varphi^2}{2h_t}, \frac{\varphi^2 - \varphi^1}{2h_x} + \frac{\varphi^3 - \varphi^4}{2h_x} \right), \quad (11.5)$$

and the discrete action becomes

$$\mathcal{A}_d[\varphi_d] = \sum_{\text{grid boxes}} L_d(\varphi^1, \varphi^2, \varphi^3, \varphi^4), \quad (11.6)$$

where $\varphi_d = \{ \{ \varphi_{i,n} \}_{i=0}^{N_x-1} \}_{n=0}^{N_t-1}$ is the discrete field. The application of Hamilton's principle

$$\left. \frac{d}{d\epsilon} \mathcal{A}_d[\varphi_d^\epsilon] \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} \sum_{\text{grid boxes}} L_d(\varphi^{1,\epsilon}, \varphi^{2,\epsilon}, \varphi^{3,\epsilon}, \varphi^{4,\epsilon}) \right|_{\epsilon=0}, \quad (11.7)$$

leads to discrete Euler-Lagrange field equations (DELFEQs) just as it lead to Euler-Lagrange equations in the continuous case. With

$$\delta \mathcal{A}_d \equiv \left. \frac{d}{d\epsilon} \mathcal{A}_d[\varphi_d^\epsilon] \right|_{\epsilon=0} \quad \text{and} \quad \delta \varphi_{i,n} \equiv \left. \frac{d}{d\epsilon} \varphi_{i,n}^\epsilon \right|_{\epsilon=0}, \quad (11.8)$$

the variation of the action can be written as

$$\delta \mathcal{A}_d = \sum_{\text{grid boxes}} \frac{\partial \mathcal{L}_d}{\partial \varphi^a}(\varphi^1, \varphi^2, \varphi^3, \varphi^4) \cdot \delta \varphi^a \quad (1 \leq a \leq 4). \quad (11.9)$$

As the variation of the action has to vanish for each $\delta\varphi_{i,n}$ on the spacetime grid, it is sufficient to consider the contributions of $\delta\mathcal{A}_d$ that are multiplied by the variation of φ at a given grid point (i, n)

$$\begin{aligned}\delta\mathcal{A}_d = & \dots + \frac{\partial L_d}{\partial\varphi^1}(\varphi_{i,n}, \varphi_{i+1,n}, \varphi_{i+1,n+1}, \varphi_{i,n+1}) \cdot \delta\varphi_{i,n} + \dots \\ & \dots + \frac{\partial L_d}{\partial\varphi^2}(\varphi_{i-1,n}, \varphi_{i,n}, \varphi_{i,n+1}, \varphi_{i-1,n+1}) \cdot \delta\varphi_{i,n} + \dots \\ & \dots + \frac{\partial L_d}{\partial\varphi^3}(\varphi_{i-1,n-1}, \varphi_{i,n-1}, \varphi_{i,n}, \varphi_{i-1,n}) \cdot \delta\varphi_{i,n} + \dots \\ & \dots + \frac{\partial L_d}{\partial\varphi^4}(\varphi_{i,n-1}, \varphi_{i+1,n-1}, \varphi_{i+1,n}, \varphi_{i,n}) \cdot \delta\varphi_{i,n} + \dots = 0. \quad (11.10)\end{aligned}$$

In total there are four such contributions, originating from the Lagrangian densities L_d of the four squares that touch the point (i, n) as is depicted in Fig. 11.2. The sum of the factors of $\delta\varphi_{i,n}$ corresponds to the discrete Euler-Lagrange field equations,

$$\begin{aligned}0 = & \frac{\partial L_d}{\partial\varphi^1}(\varphi_{i,n}, \varphi_{i+1,n}, \varphi_{i+1,n+1}, \varphi_{i,n+1}) + \frac{\partial L_d}{\partial\varphi^2}(\varphi_{i-1,n}, \varphi_{i,n}, \varphi_{i,n+1}, \varphi_{i-1,n+1}) \\ & + \frac{\partial L_d}{\partial\varphi^3}(\varphi_{i-1,n-1}, \varphi_{i,n-1}, \varphi_{i,n}, \varphi_{i-1,n}) + \frac{\partial L_d}{\partial\varphi^4}(\varphi_{i,n-1}, \varphi_{i+1,n-1}, \varphi_{i+1,n}, \varphi_{i,n}). \quad (11.11)\end{aligned}$$

Example: Wave Equation

The continuous Lagrangian for the wave equations is

$$L(u_t(t, x), u_x(t, x)) = \frac{1}{2} \left(\frac{\partial u}{\partial t}(t, x) \right)^2 - \frac{1}{2} \left(\frac{\partial u}{\partial x}(t, x) \right)^2. \quad (11.12)$$

A discretisation with the midpoint rule (11.4) leads to the discrete Lagrangian

$$L_d(u^1, u^2, u^3, u^4) = \frac{1}{2} \left(\frac{u^4 - u^1}{2h_t} + \frac{u^3 - u^2}{2h_t} \right)^2 - \frac{1}{2} \left(\frac{u^2 - u^1}{2h_x} + \frac{u^3 - u^4}{2h_x} \right)^2. \quad (11.13)$$

The four contributions to the discrete Euler-Lagrange field equations (11.11) are

$$\begin{aligned}\frac{\partial L_d}{\partial u^1}(u_{i,n}, u_{i+1,n}, u_{i+1,n+1}, u_{i,n+1}) = & -\frac{u_{i,n+1} - u_{i,n}}{4h_t^2} - \frac{u_{i+1,n+1} - u_{i+1,n}}{4h_t^2} \\ & + \frac{u_{i+1,n} - u_{i,n}}{4h_x^2} + \frac{u_{i+1,n+1} - u_{i,n+1}}{4h_x^2}, \quad (11.14a)\end{aligned}$$

$$\begin{aligned}\frac{\partial L_d}{\partial u^2}(u_{i-1,n}, u_{i,n}, u_{i,n+1}, u_{i-1,n+1}) = & -\frac{u_{i-1,n+1} - u_{i-1,n}}{4h_t^2} - \frac{u_{i,n+1} - u_{i,n}}{4h_t^2} \\ & - \frac{u_{i,n} - u_{i-1,n}}{4h_x^2} - \frac{u_{i,n+1} - u_{i-1,n+1}}{4h_x^2}, \quad (11.14b)\end{aligned}$$

$$\begin{aligned}\frac{\partial L_d}{\partial u^3}(u_{i-1,n-1}, u_{i,n-1}, u_{i,n}, u_{i-1,n}) = & +\frac{u_{i-1,n} - u_{i-1,n-1}}{4h_t^2} + \frac{u_{i,n} - u_{i,n-1}}{4h_t^2} \\ & - \frac{u_{i,n-1} - u_{i-1,n-1}}{4h_x^2} - \frac{u_{i,n} - u_{i-1,n}}{4h_x^2}, \quad (11.14c)\end{aligned}$$

$$\begin{aligned} \frac{\partial L_d}{\partial u^4}(u_{i,n-1}, u_{i+1,n-1}, u_{i+1,n}, u_{i,n}) = & + \frac{u_{i,n} - u_{i,n-1}}{4h_t^2} + \frac{u_{i+1,n} - u_{i+1,n-1}}{4h_t^2} \\ & + \frac{u_{i+1,n-1} - u_{i,n-1}}{4h_x^2} + \frac{u_{i+1,n} - u_{i,n}}{4h_x^2}. \end{aligned} \quad (11.14d)$$

Summing up all these terms, the discrete wave equation is obtained

$$\begin{aligned} & \frac{u_{i-1,n+1} - 2u_{i-1,n} + u_{i-1,n-1}}{4h_t^2} + 2 \frac{u_{i,n+1} - 2u_{i,n} + u_{i,n-1}}{4h_t^2} + \frac{u_{i+1,n+1} - 2u_{i+1,n} + u_{i+1,n-1}}{4h_t^2} = \\ & = \frac{u_{i+1,n+1} - 2u_{i,n+1} + u_{i-1,n+1}}{4h_x^2} + 2 \frac{u_{i+1,n} - 2u_{i,n} + u_{i-1,n}}{4h_x^2} + \frac{u_{i+1,n-1} - 2u_{i,n-1} + u_{i-1,n-1}}{4h_x^2}. \end{aligned} \quad (11.15)$$

This clearly is a discrete version of the continuous wave equation

$$\frac{\partial^2 u}{\partial t^2}(t, x) = \frac{\partial^2 u}{\partial x^2}(t, x),$$

with the following stencil

$$\frac{1}{4h_t^2} \begin{bmatrix} 1 & 2 & 1 \\ -2 & -4 & -2 \\ 1 & 2 & 1 \end{bmatrix} u = \frac{1}{4h_x^2} \begin{bmatrix} 1 & -2 & 1 \\ 2 & -4 & 2 \\ 1 & -2 & 1 \end{bmatrix} u. \quad (11.16)$$

We observe that the derivative with respect to one direction is averaged in the other direction, i.e., the time derivative is averaged over three neighbouring points in space, and the spatial derivative is averaged over three neighbouring points in time. This averaging of derivatives is a common feature often found in variational integrators of field theories. It appears to be one of the decisive features that account for the superior performance of variational integrators.

11.1 Discrete Jet Bundles

In order to derive a discrete version of Hamilton's action principle, we proceed in three steps. In this section, we define discrete analogues of the base space X , the configuration space Y , and the jet bundles J^1Y and J^2Y . In the next section, we discretise the Lagrangian and the action functional, and finally, we work out the discrete action principle.

The continuous base space X is replaced by its discrete analogue X_d , a bounded subset $X_d \subset \mathbb{Z}^{n+1}$ which corresponds to a grid of points in X . In what follows we assume X to be two-dimensional and choose an equidistant rectangular discretisation like it is depicted in Figure a. The theory is easily applicable to other types of grids as well, e.g., triangular as in Figure b, hexagonal as in Figure c, or even staggered or irregular ones.

The coordinates on the discrete base space $X_d \subset \mathbb{Z} \times \mathbb{Z}$ are denoted (i, j) and assumed to take values $i \in \{1, \dots, N_0\}$ and $j \in \{1, \dots, N_1\}$, respectively, where N_0 and N_1 are the number of points for each dimension. This corresponds to a grid of points $x_{i,j} = (ih, jh)$ in X with, for simplicity, the same step size h in both directions. Then

$$X_d \cong \{(ih, jh) \in X \mid i = 1, \dots, N_0, j = 1, \dots, N_1\}. \quad (11.17)$$

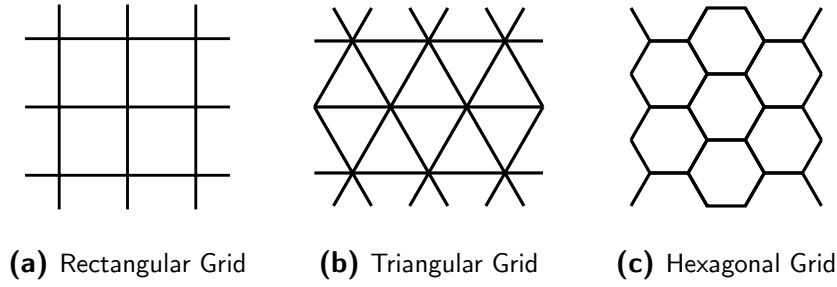


Fig. 11.3: Different regular grids.

The discrete configuration space is defined as the cartesian product

$$Y_d = X_d \times F, \quad (11.18)$$

where F is the same as in the continuous case and we have an analogous projection

$$\begin{aligned} \pi_d : Y_d &\rightarrow X_d, \\ (y_{i,j}) &\mapsto (i, j). \end{aligned} \quad (11.19)$$

Coordinates of Y_d are denoted $y_{i,j}^a$ with $1 \leq a \leq \dim F$. The coordinates of the base point (i, j) are already implied and therefore not specified separately. While coordinates on X_d and Y_d are defined point-wise, coordinates on $J^1 Y_d$ will be defined grid-cell-wise. We therefore introduce the following abstract but convenient notation. A square \square on X_d is an ordered quadruplet

$$\square = ((i, j), (i, j+1), (i+1, j+1), (i+1, j)), \quad (11.20)$$

defining a primal grid cell. The set of such cells on X_d is denoted X^\square . Vertices \square^l of a square \square with $1 \leq l \leq 4$ are counted counter-clockwise from the bottom left (c.f. Figure a), namely,

$$\square^1 = (i, j), \quad \square^2 = (i, j+1), \quad \square^3 = (i+1, j+1), \quad \square^4 = (i+1, j). \quad (11.21)$$

On a quadrilateral grid, the first jet bundle of Y_d becomes [53]

$$J^1 Y_d = X^\square \times F^4, \quad (11.22)$$

with coordinates given by

$$\{(\square, y_{\square^l}^a) \mid \square \in X^\square, y_{\square^l}^a \in \mathbb{R}, 1 \leq l \leq 4, 1 \leq a \leq \dim F\}. \quad (11.23)$$

This implies that if $\square^1 = (i, j)$, then we have

$$y_{\square^1} = y_{i,j}, \quad y_{\square^2} = y_{i,j+1}, \quad y_{\square^3} = y_{i+1,j+1}, \quad y_{\square^4} = y_{i+1,j}. \quad (11.24)$$

A section of Y_d , representing a discrete field, is a map $\varphi_d : X_d \rightarrow Y_d$ such that $\pi \circ \varphi_d = \text{id}_{X_d}$. The components of a discrete field φ_d at the vertices (11.21) of a specific square are

$$\varphi_{\square^1} = \varphi_d(\square^1), \quad \varphi_{\square^2} = \varphi_d(\square^2), \quad \varphi_{\square^3} = \varphi_d(\square^3), \quad \varphi_{\square^4} = \varphi_d(\square^4), \quad (11.25)$$

as depicted in Figure b. The discrete first jet prolongation of a discrete field φ_d is a map $j^1 \varphi_d : X^\square \rightarrow J^1 Y_d$, defined as

$$j^1 \varphi_d(\square) = (\square, \varphi_{\square^1}, \varphi_{\square^2}, \varphi_{\square^3}, \varphi_{\square^4}). \quad (11.26)$$

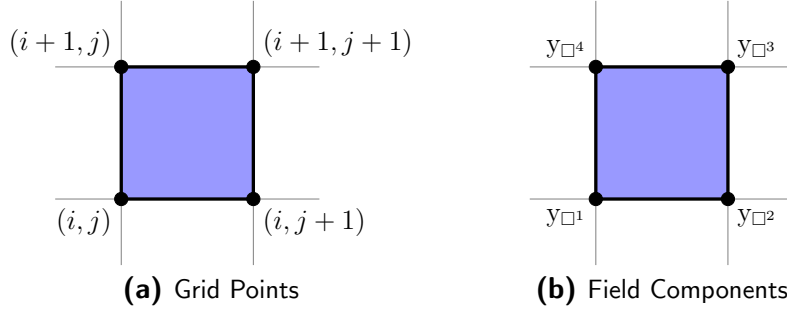


Fig. 11.4: Vertices of a primal grid cell in a two-dimensional rectangular grid and field components at those vertices.

This contains all the information necessary to define discrete first-order derivatives.

We will see that the discrete Euler-Lagrange equations are living on J^2Y_d , i.e., the second jet bundle of Y_d , similar to the continuous case (see [45] for another discussion of discrete second order jet bundles). Coordinates on J^2Y_d will be defined on a quadruple of cells \boxplus , namely those cells \square in X^\square which share a common vertex. The cells \square_m of \boxplus with $1 \leq m \leq 4$ are counted counter-clockwise from the bottom left, so that

$$\boxplus = \{\square_1, \square_2, \square_3, \square_4 \in X^\square \mid \square_1^3 = \square_2^4 = \square_3^1 = \square_4^2\}. \quad (11.27)$$

The set of all such quadruples on X_d is denoted by X^\boxplus . Vertices \boxplus^l of a quadruple \boxplus with $1 \leq l \leq 9$ are counted row-wise from bottom left to top right, namely,

$$\begin{aligned} \boxplus^1 &= (i-1, j-1), & \boxplus^2 &= (i-1, j), & \boxplus^3 &= (i-1, j+1), \\ \boxplus^4 &= (i, j-1), & \boxplus^5 &= (i, j), & \boxplus^6 &= (i, j+1), \\ \boxplus^7 &= (i+1, j-1), & \boxplus^8 &= (i+1, j), & \boxplus^9 &= (i+1, j+1). \end{aligned}$$

On a quadrilateral grid, the second jet bundle of Y_d can be identified with

$$J^2Y_d = X^\boxplus \times F^9, \quad (11.28)$$

with coordinates given by

$$\{(\boxplus, y_{\boxplus^l}^a) \mid \boxplus \in X^\boxplus, y_{\boxplus^l}^a \in \mathbb{R}, 1 \leq l \leq 9, 1 \leq a \leq \dim F\}, \quad (11.29)$$

in analogy with (11.23). The second jet prolongation of a discrete field φ_d is a map $j^2\varphi_d : X^\boxplus \rightarrow J^2Y_d$, defined as

$$j^2\varphi_d(\boxplus) = (\boxplus, \varphi_{\boxplus^1}, \varphi_{\boxplus^2}, \varphi_{\boxplus^3}, \varphi_{\boxplus^4}, \varphi_{\boxplus^5}, \varphi_{\boxplus^6}, \varphi_{\boxplus^7}, \varphi_{\boxplus^8}, \varphi_{\boxplus^9}). \quad (11.30)$$

Similar to the continuous case, J^2Y_d can also be defined via iteration as the first jet bundle of J^1Y_d . If we write coordinates on $J^1(J^1Y_d)$ as

$$\{(\boxplus, \square_m, y_{\square_m^l}^a) \mid \boxplus \in X^\boxplus, \square_m \in \boxplus, y_{\square_m^l}^a \in \mathbb{R}, 1 \leq l, m \leq 4, 1 \leq a \leq \dim F\}, \quad (11.31)$$

then J^2Y_d consists of all elements of $J^1(J^1Y_d)$, which satisfy

$$y_{\square_1^3}^a = y_{\square_2^4}^a = y_{\square_3^1}^a = y_{\square_4^2}^a, \quad y_{\square_1^2}^a = y_{\square_2^1}^a, \quad y_{\square_2^3}^a = y_{\square_3^2}^a, \quad y_{\square_3^4}^a = y_{\square_4^3}^a, \quad y_{\square_4^1}^a = y_{\square_1^4}^a, \quad (11.32)$$

for all a , which in our construction is always guaranteed due to (11.24) and (11.27). Therefore, J^2Y_d can be identified with $J^1(J^1Y_d)$, unlike the continuous case, where J^2Y is strictly embedded into $J^1(J^1Y)$.

11.2 Discrete Action Principle

The discretisation of the Lagrangian is based on the observation that the continuous action functional can be written as

$$\mathcal{A}[\varphi] = \sum_{\square \in X} \int_{\text{Vol}(\square)} L(j^1 \varphi) d^{n+1}x, \quad (11.33)$$

where $\text{Vol}(\square) \subset X$ is the physical domain enclosed by \square . The integral in (11.33) is approximated by a function of values of φ_d in four different points in the spacetime grid, which corresponds to the discrete jet prolongation defined in (11.26). This is the discrete Lagrangian L_d , i.e.,

$$\int_{\text{Vol}(\square)} L(j^1 \varphi) d^{n+1}x \approx L_d(j^1 \varphi_d(\square)) = L_d(\square, \varphi_{\square^1}, \varphi_{\square^2}, \varphi_{\square^3}, \varphi_{\square^4}). \quad (11.34)$$

The action functional (11.33) is then approximated by

$$\mathcal{A}_d[\varphi_d] = \sum_{\square \in X} L_d(j^1 \varphi_d(\square)), \quad (11.35)$$

which can also be written explicitly as

$$\mathcal{A}_d[\varphi_d] = \sum_{i=1}^{N_0-1} \sum_{j=1}^{N_1-1} L_d(\varphi_{i,j}, \varphi_{i,j+1}, \varphi_{i+1,j+1}, \varphi_{i+1,j}), \quad (11.36)$$

but for most of our derivations the abstract notation is more practical.

Specifically, the discrete Lagrangian is obtained by introducing a quadrature rule (e.g., trapezoidal, midpoint, Simpson) to approximate the integral in (11.34) as well as approximations of the fields and their derivatives. In the spirit of the Veselov discretisation [75, 76, 60, 53], we will use the midpoint rule and first-order finite differences. This entails that the continuous fields in the Lagrangian are replaced with averages of field values at the four vertices of the grid cell \square , i.e.,

$$y^a \rightarrow \frac{1}{4} (y_{\square^1}^a + y_{\square^2}^a + y_{\square^3}^a + y_{\square^4}^a) \equiv \bar{y}^a(\square). \quad (11.37)$$

There are two possibilities for the definition of each of the derivatives. With reference to Figure b, let the vertical dimension correspond to x^0 (time) and the horizontal dimension to x^1 (space). Then ∂_0 can be defined along the left as well as along the right edge of the grid cell. Similarly, ∂_1 can be defined along the upper as well as along the lower edge. Best results are usually obtained for the most symmetric discretisation of the Lagrangian. Therefore we use the average of the respective options and replace the derivatives in the Lagrangian according to

$$z_0^a \rightarrow \frac{1}{2} \left(\frac{y_{\square^4}^a - y_{\square^1}^a}{h} + \frac{y_{\square^3}^a - y_{\square^2}^a}{h} \right) \equiv \bar{z}_0^a(\square), \quad (11.38)$$

$$z_1^a \rightarrow \frac{1}{2} \left(\frac{y_{\square^2}^a - y_{\square^1}^a}{h} + \frac{y_{\square^3}^a - y_{\square^4}^a}{h} \right) \equiv \bar{z}_1^a(\square). \quad (11.39)$$

At last, in order to obtain the discrete equations of motion, we only need to apply a discrete version of Hamilton's principle of stationary action. The vertical transformation σ^ϵ is discretised in the same way as the fields φ , by considering its values over points (i, j) of the discrete base

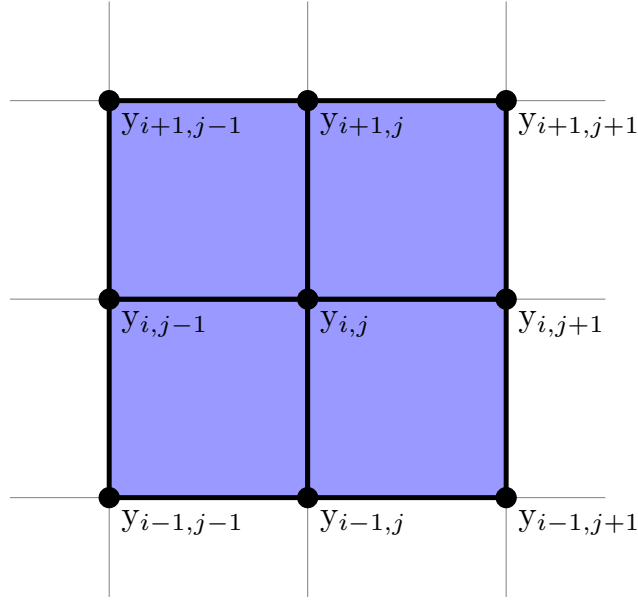


Fig. 11.5: Contributions to the discrete Euler-Lagrange field equations. The derivatives of the discrete Lagrangian at the highlighted grid cells with respect to $y_{i,j}$ correspond to the terms in equation (11.43).

space X_d , i.e., we replace $\sigma^\epsilon(x, y)$ with $\sigma_d^\epsilon = (\sigma_{i,j}^\epsilon(y_{i,j}))$. The generating vector field is computed as in the continuous case, but on grid points only,

$$\eta_{i,j}^a = \left. \frac{d(\sigma_{i,j}^\epsilon)^a}{d\epsilon} \right|_{\epsilon=0}. \quad (11.40)$$

The discrete version of Hamilton's action principle then reads

$$\left. \frac{d}{d\epsilon} \mathcal{A}_d[\sigma_d^\epsilon \circ \varphi_d] \right|_{\epsilon=0} = 0 \quad \text{for every } \sigma_d^\epsilon. \quad (11.41)$$

The explicit computation of (11.41) leads to

$$\begin{aligned} \left. \frac{d}{d\epsilon} \mathcal{A}_d[\sigma_d^\epsilon \circ \varphi_d] \right|_{\epsilon=0} &= \sum_{\square \in X_\square} \left. \frac{d}{d\epsilon} L_d(j^1 \varphi_d^\epsilon(\square)) \right|_{\epsilon=0} \\ &= \sum_{\square \in X_\square} \sum_{l=1}^4 \frac{\partial L_d}{\partial y_{\square^l}^a} (j^1 \varphi_d(\square)) \cdot \eta_{\square^l}^a(\varphi_{\square^l}). \end{aligned} \quad (11.42)$$

As the variation of the action has to vanish for each $\eta_{i,j}^a$ on the spacetime grid independently, it is sufficient to consider only those contributions that are multiplied with the vector field at a fixed grid point (i, j) . In total there are four such contributions (see Figure 11.5),

$$\begin{aligned} \left. \frac{d}{d\epsilon} \mathcal{A}_d[\sigma_d^\epsilon \circ \varphi_d] \right|_{\epsilon=0} &= \\ &\dots + \frac{\partial L_d}{\partial y_{\square^1}^a} (\varphi_{i,j}, \varphi_{i,j+1}, \varphi_{i+1,j+1}, \varphi_{i+1,j}) \cdot \eta_{i,j}^a(\varphi_{i,j}) + \dots \\ &\dots + \frac{\partial L_d}{\partial y_{\square^2}^a} (\varphi_{i,j-1}, \varphi_{i,j}, \varphi_{i+1,j}, \varphi_{i+1,j-1}) \cdot \eta_{i,j}^a(\varphi_{i,j}) + \dots \\ &\dots + \frac{\partial L_d}{\partial y_{\square^3}^a} (\varphi_{i-1,j-1}, \varphi_{i-1,j}, \varphi_{i,j}, \varphi_{i,j-1}) \cdot \eta_{i,j}^a(\varphi_{i,j}) + \dots \end{aligned}$$

$$\dots + \frac{\partial L_d}{\partial y_{\square^4}^a} \left(\varphi_{i-1,j}, \varphi_{i-1,j+1}, \varphi_{i,j+1}, \varphi_{i,j} \right) \cdot \eta_{i,j}^a(\varphi_{i,j}) + \dots = 0.$$

The variation of the discrete action vanishes, if the sum of all expressions multiplying $\eta_{i,j}^a$ vanishes identically for all (i, j) (since the $(\sigma_{i,j}^\epsilon)^a$ and therefore the $\eta_{i,j}^a$ are arbitrary). For each a , this requirement yields the discrete Euler-Lagrange field equations at (i, j) ,

$$\begin{aligned} 0 = & \frac{\partial L_d}{\partial y_{\square^1}^a} \left(\varphi_{i,j}, \varphi_{i,j+1}, \varphi_{i+1,j+1}, \varphi_{i+1,j} \right) + \frac{\partial L_d}{\partial y_{\square^2}^a} \left(\varphi_{i,j-1}, \varphi_{i,j}, \varphi_{i+1,j}, \varphi_{i+1,j-1} \right) \\ & + \frac{\partial L_d}{\partial y_{\square^3}^a} \left(\varphi_{i-1,j-1}, \varphi_{i-1,j}, \varphi_{i,j}, \varphi_{i,j-1} \right) + \frac{\partial L_d}{\partial y_{\square^4}^a} \left(\varphi_{i-1,j}, \varphi_{i-1,j+1}, \varphi_{i,j+1}, \varphi_{i,j} \right), \end{aligned} \quad (11.43)$$

which can be compactly written as an equation on the discrete second jet bundle $J^2 Y_d$, namely

$$(j^2 \varphi_d(\boxplus))^* (D_{\text{EL}}(L_d))^a = \sum_{\substack{l=1 \\ \square^l = \boxplus^5}}^4 \frac{\partial L_d}{\partial y_{\square^l}^a} (j^1 \varphi_d(\square)) = 0 \quad \text{for all } a \text{ and all } \boxplus. \quad (11.44)$$

Here, $D_{\text{EL}}(L_d)$ is the discrete Euler-Lagrange operator acting on the discrete Lagrangian L_d , which is evaluated on the prolongation $j^2 \varphi_d(\boxplus)$ as indicated by the pull-back notation. These relations define the variational integrator for a first-order Lagrangian field theory according to the Veselov discretisation of the Lagrangian as it was described above.

11.3 Discrete Noether Theorem

Following the derivation of the continuous theory from the previous section, we consider vertical transformations $\sigma_{i,j}^\epsilon(y_{i,j})$ and define

$$\varphi_{i,j}^\epsilon = \sigma_{i,j}^\epsilon \circ \varphi_{i,j} \quad \text{with} \quad \sigma_{i,j}^\epsilon|_{\epsilon=0} = \text{id} \quad \text{and} \quad \eta_{i,j}^a = \left. \frac{d(\sigma_{i,j}^\epsilon)^a}{d\epsilon} \right|_{\epsilon=0}. \quad (11.45)$$

The transformation $\sigma_{i,j}^\epsilon$ is a symmetry for the discrete Lagrangian (11.34) if

$$L_d(j^1 \varphi_d^\epsilon(\square)) = L_d(j^1 \varphi_d(\square)), \quad (11.46)$$

which is equivalent to the infinitesimal symmetry condition

$$\left. \frac{d}{d\epsilon} L_d(j^1 \varphi_d^\epsilon(\square)) \right|_{\epsilon=0} = \sum_{l=1}^4 \frac{\partial L_d}{\partial y_{\square^l}^a} (j^1 \varphi_d(\square)) \cdot \eta_{\square^l}^a(\varphi_{\square^l}) = 0. \quad (11.47)$$

On each grid cell \square we can define four discrete momentum maps in analogy to (10.126),

$$(j^1 \varphi_d(\square))^* J_{\square^l} = \frac{\partial L_d}{\partial y_{\square^l}^a} (j^1 \varphi_d(\square)) \cdot \eta_{\square^l}^a(\varphi_{\square^l}), \quad l \in \{1, 2, 3, 4\}. \quad (11.48)$$

Instead of two components of J , corresponding to the coordinates of the base space, we now have four contributions, corresponding to the vertices of a grid cell. With that, we can write the discrete symmetry condition (11.47) as

$$J_{\square^1} + J_{\square^2} + J_{\square^3} + J_{\square^4} = 0, \quad \text{for every } \square \in X^\square. \quad (11.49)$$

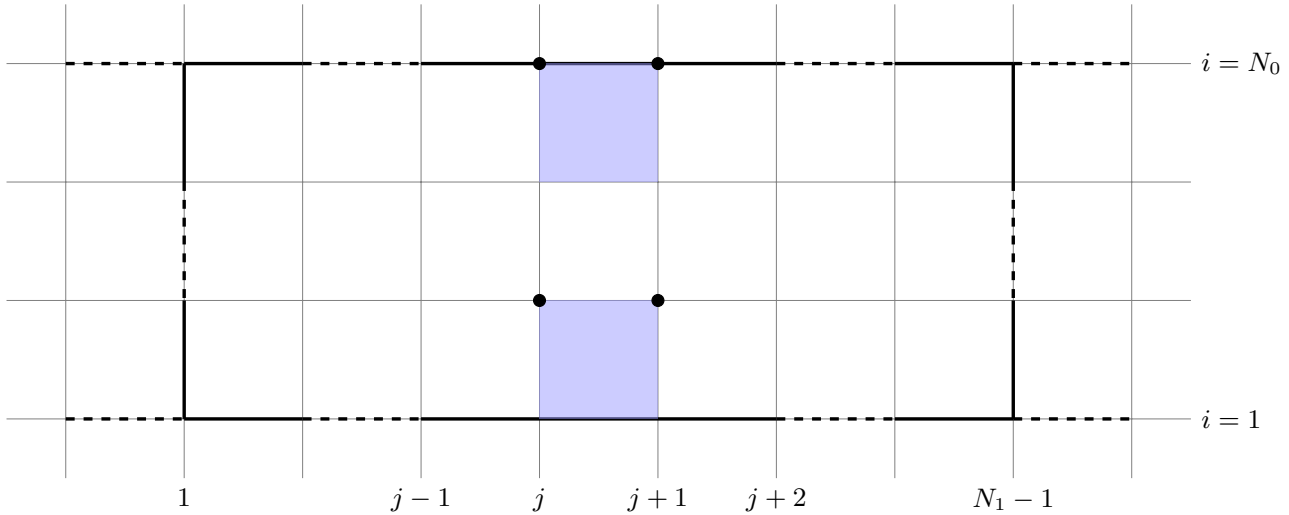


Fig. 11.6: Contributions to the discrete Noether theorem.

In addition to (11.48), we define some explicit shorthand notation that will become useful in the following derivation,

$$J_{i,j}^1 = \frac{\partial L_d}{\partial y_{\square^1}^a}(\varphi_{i,j}, \varphi_{i,j+1}, \varphi_{i+1,j+1}, \varphi_{i+1,j}) \cdot \eta_{i,j}^a(\varphi_{i,j}), \quad (11.50a)$$

$$J_{i,j}^2 = \frac{\partial L_d}{\partial y_{\square^2}^a}(\varphi_{i,j}, \varphi_{i,j+1}, \varphi_{i+1,j+1}, \varphi_{i+1,j}) \cdot \eta_{i,j+1}^a(\varphi_{i,j+1}), \quad (11.50b)$$

$$J_{i,j}^3 = \frac{\partial L_d}{\partial y_{\square^3}^a}(\varphi_{i,j}, \varphi_{i,j+1}, \varphi_{i+1,j+1}, \varphi_{i+1,j}) \cdot \eta_{i+1,j+1}^a(\varphi_{i+1,j+1}), \quad (11.50c)$$

$$J_{i,j}^4 = \frac{\partial L_d}{\partial y_{\square^4}^a}(\varphi_{i,j}, \varphi_{i,j+1}, \varphi_{i+1,j+1}, \varphi_{i+1,j}) \cdot \eta_{i+1,j}^a(\varphi_{i+1,j}). \quad (11.50d)$$

In order to derive the discrete conservation law, we follow the same argument as in the continuous case. If the Lagrangian is invariant under a given vertical transformation, then the action is also invariant under this transformation, namely,

$$\left. \frac{d}{d\epsilon} \mathcal{A}_d[\varphi_d^\epsilon] \right|_{\epsilon=0} = 0, \quad (11.51)$$

which becomes

$$\begin{aligned} \left. \frac{d}{d\epsilon} \mathcal{A}_d[\varphi_d^\epsilon] \right|_{\epsilon=0} &= \sum_{\square \in X^\square} \sum_{l=1}^4 \frac{\partial L_d}{\partial y_{\square^l}^a}(\mathbf{j}^1 \varphi_d(\square)) \cdot \eta_{\square^l}^a(\varphi_{\square^l}) \\ &= \sum_{\square \in X^\square} \sum_{l=1}^4 (\mathbf{j}^1 \varphi_d(\square))^* J_{\square^l} = 0. \end{aligned} \quad (11.52)$$

Those contributions to the sum that originate from interior points vanish in virtue of the discrete Euler-Lagrange field equations (11.43). Specifically,

$$J_{i,j}^1 + J_{i,j-1}^2 + J_{i-1,j-1}^3 + J_{i-1,j}^4 = (\mathbf{j}^2 \varphi_d(\boxplus))^* (\mathbf{D}_{\text{EL}}(L_d))_{i,j}^a \cdot \eta_{i,j}^a(\varphi_{i,j}) = 0, \quad (11.53)$$

so that only boundary cells contribute to (11.52), c.f. Figure (11.6). For simplicity, we will assume periodic boundary conditions in the space-like variable, then the only contribution comes from the

boundary of the time-like variable,

$$0 = \sum_{j=1}^{N_1-1} \left[J_{1,j}^1 + J_{1,j-1}^2 + J_{N_0-1,j-1}^3 + J_{N_0-1,j}^4 \right]. \quad (11.54)$$

Using the discrete symmetry condition (11.49) to replace the first two terms as well as the periodicity of the spatial domain, we obtain the discrete conservation law

$$\sum_{j=1}^{N_1-1} \left[J_{1,j}^3 + J_{1,j}^4 \right] = \sum_{j=1}^{N_1-1} \left[J_{N_0-1,j}^3 + J_{N_0-1,j}^4 \right], \quad (11.55)$$

see Figure 11.6. Since the number of timesteps N_0 is arbitrary, this is equivalent to

$$\mathcal{J}_d = \sum_{\substack{j=1 \\ \square^1=(i,j)}}^{N_1-1} \left[J_{\square^3}(j^1 \varphi_d(\square)) + J_{\square^4}(j^1 \varphi_d(\square)) \right] = \text{const. for all } i, \quad (11.56)$$

in analogy to the continuous Noether charge. This proves that variational integrators preserve discrete invariants \mathcal{J}_d to machine accuracy¹.

Discrete Divergence Symmetries

We can generalise the discrete Noether theorem in a similar way as we did with the continuous Noether theorem for divergence symmetries. In analogy to the continuous symmetry condition for divergence symmetries, we rewrite the discrete symmetry condition (11.49) as

$$J_{\square^1} + J_{\square^2} + J_{\square^3} + J_{\square^4} = B_{\square^1} + B_{\square^2} + B_{\square^3} + B_{\square^4}. \quad (11.57)$$

Making no assumption on the B_{\square^i} , equation (11.54) takes the form

$$\begin{aligned} \sum_{j=1}^{N_1-1} \left[J_{1,j}^1 + J_{1,j-1}^2 - B_{1,j}^1 - B_{1,j-1}^2 + J_{N_0-1,j-1}^3 + J_{N_0-1,j}^4 - B_{N_0-1,j-1}^3 - B_{N_0-1,j}^4 \right] = \\ = \sum_{i=2}^{N_0-1} \sum_{j=1}^{N_1-1} \left[B_{i,j}^1 + B_{i,j-1}^2 + B_{i-1,j-1}^3 + B_{i-1,j}^4 \right]. \end{aligned} \quad (11.58)$$

We conclude, that we have the discrete equivalent of a divergence symmetry, if the sum of all $B_{i,j}^l$ in the interior of X_d vanishes,

$$\sum_{i=2}^{N_0-1} \sum_{j=1}^{N_1-1} \left[B_{i,j}^1 + B_{i,j-1}^2 + B_{i-1,j-1}^3 + B_{i-1,j}^4 \right] = 0, \quad (11.59)$$

such that only the fluxes at the boundaries of X_d contribute to (11.58). Then, the generalised Noether charge (11.56) becomes

$$\mathcal{J}_d = \sum_{\substack{j=1 \\ \square^1=(i,j)}}^{N_1-1} \left[J_{\square^3}(j^1 \varphi_d(\square)) + J_{\square^4}(j^1 \varphi_d(\square)) - B_{\square^3}(j^1 \varphi_d(\square)) - B_{\square^4}(j^1 \varphi_d(\square)) \right] = \text{const. for all } i, \quad (11.60)$$

in correspondence with the continuous Noether current for divergence symmetries.

¹In practice, many variational integrators require the solution of nonlinear algebraic equations. In that case, the accuracy to which the invariants are preserved will generally depend on the accuracy of the nonlinear solver.

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