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Further Analysis of Cellular Pathways

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Abstract

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Chapter 1

Introduction

Paolo Dini, Alastair J Munro and Ferenc Ruzsnavszky

This deliverable collects the mathematics, biology, and physics work of the final year of the project around the central themes of non-linear coupling and dynamical stability.

In this introduction we revisit the basic definitions of equilibrium and stability for closed and open systems. We also summarize some work done on the Calcium cycle of cardiac myocytes that has not yet been reported in other BIOMICS deliverables. Although this system exhibits oscillations and is stable, the available mathematical model of the membrane potential turned out to be too simplistic to serve as a starting point for this very complex system. By the same token, a more faithful mathematical model is too difficult to analyse using the Lie group approach. Thus, although it was very helpful as an example through which the Abstract State Machine (ASM) concepts could be explained to the biologists and physicists, it did not seem fruitful to pursue it further.

Chapter 2 provides a wide-ranging discussion of invariants of the motion of dynamical systems and of a stochastic modelling approach for the meta-stable behaviour of metabolic systems in terms of their 'quasi-potential', from a mathematical physics perspective. Chapter 3 studies ODEs of arbitrary order that admit a given symmetry group. Chapter 4 derives the Lie group for a specific 2nd-order equation modelling a biological system, the Fitzhugh-Nagumo model of nerve conduction [27, Chapter 7, p. 177].

Second-order systems only admit a finite-dimensional symmetry group, and therefore are easier to characterize completely than first-order systems. First-order systems admit an infinite-dimensional Lie group, and therefore it may be hard to find symmetries for them. On the other hand, if the system is re-written as a 2nd-order one, one has a chance of finding all its symmetries, and then "pull the symmetries back" to the 1st-order system, and get a solution. The relevance of 2nd-order systems, which are also the focus of Chapter 2, arises from the Smoluchowski-Kramers approximation of Langevin's equation for Brownian motion [10], in which the small mass of the Brownian particle justifies neglecting the highest-order derivative or inertia term. As a result, the original force field acts on a diffusion system, which is analogous to the dissipative 1st-order systems of ODEs modelling metabolic pathways and whose meta-stable properties are studied through the quasi-potential [18, 51].

In the next section we summarize briefly the reasons that led us to abandon the Calcium cycle from further analysis, in spite of the fact that as a biological example it served as a useful meeting point between the computer scientists, the biologists, and the physical scientists. In Section 1.2 we provide a context from which the concept of dynamical stability has emerged, as an introduction to Chapter 2.

1.1 The Goldman Equation in the Calcium Cycle of Cardiac Myocytes

In [42] we derived the Goldman equation for the voltage across the membrane of cardiac cells, whose periodic contractions are driven by oscillations in the Calcium concentration levels in the cytoplasm:

$$[2P_{Ca}Ca_{in} + P_{Na}Na_{in} + P_K K_{in}]e^{2a} + [P_{Na}(Na_{in} - Na_{out}) + P_K(K_{in} - K_{out})]e^{a} \\ -[2P_{Ca}Ca_{out} + P_{Na}Na_{out} + P_K K_{out}] = 0. \qquad (1.1)$$

The physically meaningful root is e^a, such that the voltage is given by

$$V = \frac{R\mathbb{T}}{F} \ln e^a = \frac{R\mathbb{T}}{F} a, \tag{1.2}$$

where R is the universal gas constant, F is Faraday's constant, and $\mathbb{T}$ is the absolute temperature in Kelvin. This equation relates the ion concentrations on either sides of the cell membrane to the voltage required to achieve a zero *total* net ion current across the membrane. This is just a generalization to more than one ion of the Nerst potential, i.e. the potential needed to counteract the chemical potential due to a difference in ion concentration across the membrane and achieve zero net ion flow. In the case of two or more ions the total net current over all the ions is still zero, but the (average) current of each ion is not necessarily zero. In other words, the Goldman equation becomes an integral constraint.

It is worth remarking that in experimental conditions normally the voltage is set ('clamped') at some fixed value and the Goldman equation is used to predict or verify the ion concentrations just inside the cell. Also, the supply of ions outside the cell is so great that the external concentrations do not change during the Calcium cycle, so all the outside variables are constant.

In [42] we stated that the execution of the Abstract State Machine (ASM) model of the Calcium cycle developed in that report involves specifying the quantities of ions that need to be moved by the currents across the cell membrane and in and out of the sarcoplasmic reticulum. Knowing the concentration levels of the three ions on the two sides of the membrane would then enable us to calculate the voltage, as above. In other words, the plan was to use the Goldman equation in the opposite way to how it is normally used in experimental situations.

If we define the state of the system as a point in "phase space" ($\mathbb{R}^n$, where $n =$ number of different ion species), then the behaviour of the system is a set of tuples of ion concentrations. Our thinking was that, although the values of the ion concentrations would be coming from experimental data – reducing the above model to little more than a curve-fitting exercise – it was still potentially fruitful to run the model for many conditions in order to develop, numerically, a function of the ion concentrations (i.e., $\mathbb{R}^n \to \mathbb{R}$) that could have shown the stable periodic behaviour of the system as the minimum of a time-dependent potential.

Unfortunately, we had neglected an important feature of this system. Due to the obvious need to minimize energy usage of the heart muscle, which never stops beating, the quantity of ions that are actually moved across the membrane is tiny. What has an even greater effect on the value of the voltage, and therefore on the formation and shape of the voltage pulse, is the variation of the permeabilities, shown in the above equations as P_x, where x stands for the names of the different ions. The permeabilities, in turn, depend on both the voltage and on the concentrations, thereby giving rise to a strongly non-linear system in 6 coupled, dependent variables. Such a system is well beyond the ability of the relatively simple Goldman equation to model it.

Therefore, this branch of research activity was stopped at this point. It had in any case already served its purpose of providing a way to relate biological and ASM concepts across the very different disciplines of biology and computer science, and had given us some conceptual examples of stable oscillatory behaviour to guide our further explorations. In particular, we kept the focus on the concept of the time-dependent potential in the next step of the research, foregrounded in the next section and discussed in more detail in Chapter 2.

1.2 Equilibrium, the Balance of Nature Fallacy, and Dynamical Stability

> The Balance of Nature is a theory that proposes that ecological systems are usually in a stable equilibrium, which is to say that a small change in some particular parameter will be corrected by some negative feedback that will bring the parameter back to its original 'point of balance' with the rest of the system.[1]

[1] https://en.wikipedia.org/wiki/Balance_of_nature

As suggestively reported by Adam Curtis in his documentary 'The Use and Abuse of Vegetational Concepts',[2] this theory was dominant until approximately 1980, when fieldwork, undertaken as part of a project led by George van Dyne, suggested that no such balance existed. Ecosystems, it seems, will not return to some 'equilibrium' when disturbed by small- or large-scale disasters: new configurations will ensue.

Ecological population models are among the most well-studied dynamical systems, usually modelled with sets of coupled, non-linear differential equations. In BIOMICS, we are interested in studying cell metabolic and regulatory pathways because they appear to exhibit a form of stability under external perturbations that is generally associated with the state of 'health' of the organism. We wish to understand this form of stability and see whether it can be formalized as 'self-organizing behaviour' of systems in general and, in particular, of computational systems. The biochemical systems of the cell are also modelled with systems of coupled, non-linear differential equations. Although the empirical evidence that ecosystems are not 'stable' in any conventional sense of the term is by now compelling, so is the behavioural distinction between, for example, a healthy and a cancerous cell. Therefore, it would appear that the concept of stability is rather subtle and needs to be handled differently for biological systems in different contexts (e.g. over different spatial and temporal scales).

'Equilibrium' and 'steady-state' are often used interchangeably, but they are not necessarily synonymous. The configuration space of a dynamical system is the space defined by treating the dependent variables as independent dimensions. A solution of the system then becomes a curve in this space parametrized by time. In dynamical systems theory, an equilibrium point in configuration space is a point at which the rate of change of the problem variables with respect to time is zero. An isolated dissipative system that is started away from equilibrium will eventually "fall" back to the equilibrium state. The portion of the solution of an isolated system that is a function of time but that is approaching equilibrium is called the transient response.

If we characterize the state of a system as a point in configuration space, the following quotation from Crawford [11] seems helpful: 'The world is full of things that move. Their motions can broadly be categorized into two classes, according to whether the thing that is moving stays near one place or travels from one place to another'. Oscillations belong to the first class, and are characterized by three things:

- The existence of an equilibrium state
- The presence of a return force when the system is displaced from equilibrium
- The presence of an inertia that causes the system to overshoot equilibrium

The presence of a return force makes the equilibrium point *stable*. Steady state, on the other hand, indicates more generally the condition where the transient has been damped by friction. In a driven (i.e. not isolated) oscillator, the steady-state part of the solution is still a function of time, but has become periodic. The same idea applies in higher dimensions. By contrast, Newton's law can also be regarded as a condition of 'dynamical equilibrium': the motion of an accelerating mass could therefore be seen in dynamical equilibrium simply because it is consistent with $F = ma$. So, one needs to pay attention to the context in which these terms are used.

A system may have one or more stable equilibrium points, but its behaviour may still be unstable. A dynamical system is considered to be stable if external perturbations cause oscillations whose amplitude does not increase over time. It is unstable otherwise. If we regard biological organisms as complex dynamical systems and if we associate health with equilibrium, then according to this definition their ability to heal themselves would seem to make healthy organisms 'stable'. However, systems that we can model mathematically and that are stable are not capable of exhibiting complex

[2] Part 2 of the series *All Watched Over by Machines of Loving Grace*, https://en.wikipedia.org/wiki/All_Watched_Over_by_Machines_of_Loving_Grace_%28TV_series%

behaviour in any way resembling biological organisms. So, 'biological stability' must be more complex both conceptually and mathematically. Another perspective on biological stability is stability as phenomenological illusion: a system may appear to be stable on the outside but may rely on complex and locally unstable interactions on the inside. Figure 1.1 shows how the external stability of a loosely grouped system (a family of ducks) depens on a great deal of internal dynamics and communications. This is getting closer to self-organization through interactions.

Fig. 1.1: **Phenomenological stability often depends on a lot of hidden activity and internal interactions** (Source: http://www.rspb.org.uk/community/wildlife/f/13609/t/82656.aspx)

Until approximately 1980, ecology as a science was based on the assumption that ecosystems are stable: if a hurricane, or a fire, or an earthquake disturbed an ecosystem, the assumption was that after some time the ecosystem would regain its original equilibrium state: Nature was assumed to be 'in balance'. In the late 1970s, fieldwork performed by the ecologist George van Dyne, however, showed fairly convincingly that ecosystems are not in balance: a large perturbation causes an ecosystem to drift to a different configuration, potentially very different from the original. The irony is that van Dyne was in fact trying to do the opposite, to confirm the Balance of Nature theory. It is possible that the Balance of Nature fallacy originates from the fact that in (bio)chemical systems *we cannot properly talk about an inertia*. Hence the importance of time-delays in oscillating biochemical systems.

When a theory does not fit anymore, we (sometimes) generalize. A first possibility is to say that – rather than a single equilibrium point – complex non-linear systems have multiple equilibria. Systems with two or more stable equilibria are called meta-stable. The transitions between different meta-stable states result from external inputs, i.e. from interactions of the system with its environment. Biological systems appear to transition between different meta-stable states continuously, in real time, as a result of the continuous interactions between external inputs and internal components, at different length and time scales. We have tentatively called such continuously varying trajectory of meta-stable states *dynamical stability*. Dynamical stability may be a conserved quantity or a function of conserved quantities. Hence our effort to use Lie symmetries to guide the analysis (see Chapters 3 and 4). More recently, we have begun to suspect that a probabilistic/stochastic approach may be necessary to explore meta-stable systems through the 'quasi-potential', as explained in the next chapter.

Dynamical stability has interesting resonance with one of the paradoxes of evolutionary biology: if the laws of thermodynamics indicate that entropy should increase over time, then why, and how, does evolution produce increased organisation and complexity? Perhaps 'dynamical stability' is part of the answer.

Chapter 2

Dynamical Stability, Hamilton-Jacobi Theory and the Quasi-Potential

Paolo Dini, Ágnes Bonivárt and Chrystopher L. Nehaniv

2.1 Introduction

This chapter discusses two fundamental concepts in the mathematical physics of dynamical systems, the potential and the invariants of the motion. Since the invariants of the motion are very difficult to find, because finding them amounts to finding the analytical solution of the problem, the chapter spends more time with the potential. Another reason for focusing more on the potential is that, surprisingly, it can be related to stochastic models of *dissipative* biochemical systems through a probability theory formalization – the 'quasi-potential' – that is well-developed in terms of theoretical results and numerical analysis methods. The invariants of the motion, which depending on the context can also be called 'constants of motion' or 'first integrals', will nonetheless remain in the background and will make several appearances in this chapter.

The general concept of 'potentiality' of motion or action goes back to Aristotle, and acquired its classical physics meaning of 'potential energy' in the 18th Century through the work of Euler and Lagrange. The common and intuitive understanding of 'potential' can be visualized as a rigid surface upon which a ball rolls or slides under the action of gravity. Such a visualization corresponds to the mathematical statement that the net force vector acting on a (frictionless) single-particle system is the negative gradient of such a potential surface. The ball will fall towards the point of minimum height of the surface, a process that is referred to as 'minimization of potential energy', or 'minimization of energy' for short, and that at each point in time is consistent with Newton's Second Law.

In the 19th Century development of statistical physics by Boltzmann and others, the concept of potential was generalized to 'large' or thermodynamic systems, i.e. systems whose number of particles is on the order of Avogadro's number. The existence of a minimum potential energy (usually a potential energy of interaction between the particles) is in this case complemented by the evolution of the system towards its most likely configuration, a process that is known as 'maximization of entropy' and that is usually modelled as diffusion. The two processes can be combined in the minimization of the system's 'free energy', defined as the difference between the potential energy and the entropy. Other analogous 'thermodynamic potentials' can likewise be defined for systems subject to different kinds of constraints (constant volume, constant pressure, variable number of particles, etc).

The potential is also used within biology, but in a rather different way. To explain the stability of biological development, the use of the classical physics potential as a metaphor appears to have originated in 1942 with Waddington's 'canalization' [47], which was then further developed as 'epigenetic landscape' ([48], cited in [30]: 448). Canalization refers to the narrowing of the future choices of the progeny of a stem cell as it becomes increasingly specialized. In other words, the growth of a developing embryo towards a particular phenotype can be seen as the "fall" towards the minimum of a complex potential landscape whose shape is largely determined by the organism's DNA and the interaction of environmental inputs with the web of its epigenetic interdependences.

The BIOMICS project started with the assumption that a similar concept would apply to the cell's metabolic and regulatory processes, whose order-construction or order-maintenance ability is generally described as a free energy-minimization process. The free energy is provided by food, thereby implying an open-system architecture for all biological systems. Their spontaneous self-organizing properties, therefore, rely on the constant supply of free energy keeping the system away from equilibrium even while it is continuously falling towards it. Like morphogenesis, also metabolic and regulatory processes are ontogenetic, such that in both cases it seems appropriate to talk about a dynamical process evolving in a stable potential "channel" and towards a robustly stable minimum. However, whereas in the case of morphogenesis future phenotypical traits build on prior structure, thereby limiting the future range of possibilities with each step of the development process, in the case of metabolism and cell regulation the system is much more dynamic and unencumbered by a growing and increasingly rigid structure. As a consequence, sub-cellular biochemical systems are generally understood to transition between a number of possible and *different* 'meta-stable' states, each of which can be seen as a local minimum in a potential landscape.

One of the objectives of the project has been to develop the concept of meta-stability further, as 'dynamical stability', and to define it mathematically. As the project nears its end it is not clear whether we will be able to achieve a satisfactory mathematical definition of dynamical stability. At a conceptual level, it can be understood as a generalization of the meta-stable landscape in the form of a *time-dependent* meta-stable potential landscape, like the surface of a wavy sea. At the same time, however, the invariants of the motion appear to be equally important, because they can represent physical constraints that limit the region of phase space the problem variables can explore, in essence providing a step towards the solution's unique time-evolution.

At the simplest level, the constants of the motion are none other than the constants of integration of a differential problem. In the case of a single, first-order differential equation $\dot{x} = f(t, x)$, the value of the constant of integration is set by the initial condition and can also be seen as the value of the level set of a surface $\Phi(t, x)$ defined over the dependent and independent variable. Different solution curves $x(t)$, therefore, correspond to different level sets of $\Phi(t, x)$, and are in fact their projections onto the t-x plane.

The representation of solutions, however, is normally effected by defining two different kinds of space, each of which is different from the above. The *configuration space* is a space comprising only the dependent variables, such that solutions are curves $\gamma\colon \mathbb{R} \to \mathbb{R}^n$ parametrized with time, where n is the number of dependent variables. In the above example the whole solution would live *within* a single line; since this does not convey much information, for the 1-D case the usual graph of a function representation in the plane is used. Alternatively, solutions can also be represented as curves $\gamma\colon \mathbb{R} \to \mathbb{R}^{2n}$, also parametrized with time, in *phase space*, which is a space defined by the dependent variables and their first time derivatives. With this context, following [6] we distinguish between 'constants of the motion' and 'integrals of the motion' as follows:

- **Constant of the motion**: any function $C(x, \dot{x}, t)\colon \mathbb{R}^{2n+1} \to \mathbb{R}$ that is constant along any solution curve $\gamma(t)\colon \mathbb{R} \to \mathbb{R}^n$, where n is the dimension of the configuration space, or the number of dependent variables, or the number of 1st-order ordinary differential equations (ODEs).
- **Integral of the motion, or first integral**: any function $I(x, \dot{x})\colon \mathbb{R}^{2n} \to \mathbb{R}$ of the phase space variables only that is constant along any phase space orbit $\zeta(t)\colon \mathbb{R} \to \mathbb{R}^{2n}$.

Whereas every integral of motion is a constant of motion, the converse is not necessarily true since a constant of motion may depend explicitly on time. The phase space variables are usually the dependent variables and their first time derivatives.[3] In first-order systems such as the metabolic systems of interest to BIOMICS, on the other hand, phase space is composed of only the dependent variables.

When the solution is expressed as a phase space trajectory parametrized by time, it can be seen as a projection of a level set of a first integral onto the phase space: $\mathbb{R}^{2n+1} \to \mathbb{R}^{2n}$. When the solution

[3] The first time derivatives are needed because the governing equations are second-order, and the uniqueness of their solution requires the setting of initial values for their positions and velocities. The Hamiltonian formalism, upon which we rely here, further requires the use of momenta rather than velocities.

is a curve in a space defined by the dependent variables and time (configuration space plus time), it similarly lives on a level set of a constant of the motion. In this case, however, the graph of *each* dependent variable as a function of time can be obtained as a projection $\mathbb{R}^{n+2} \to \mathbb{R}^2$.

When integrals of the motion have a physical interpretation they can provide an additional level of explanation for the observed behaviour. For the purposes of the project, for example, we postulated that dynamical stability and self-organizing behaviour may be related to the integrals or the constants of the motion of the problem. Although this would probably help significantly in providing a mathematical formalization of dynamical stability, the challenge in proving this conjecture is that the mathematical models of systems that exhibit self-organizing behaviour are, in their simplest form, sets of coupled and non-linear ODEs whose solutions are immensely difficult to find.

The theory of Lie groups for the analysis of systems of ODEs has been discussed at length in previous BIOMICS reports [14, 13, 17] that are in part based on an extensive literature, e.g. [40, 25, 24, 43], and is further discussed in Chapters 3 and 4 of this report. This theory is hampered by the lack of a general method for finding the symmetries of a given system but, even more, by the fact that as systems become more complex the discovery or identification of an appropriate number of symmetries is not necessarily sufficient for finding the full analytical solution or its first integral in terms of elementary functions.

In light of the daunting difficulty of finding – or, indeed, *creating* – analytical solutions for most differential problems involving more than two 1st-order ODEs, for the past few decades research in the area of modelling dynamical – and in particular biochemical – systems has shifted towards stochastic methods. Stochastic models are appropriate for systems that are large in terms of particle number but not large enough to justify continuous ODE models. The theory of stochastic differential equations (SDEs) appears to provide a sufficiently different perspective and set of analytical tools to push our ability to analyse more complex systems than the symmetry analysis of deterministic ODEs appears to be able to achieve. In particular, we are referring to Freidlin and Wentzell's [18] theory of large deviations, which is where the concept of the quasi-potential was first introduced. The most interesting theoretical insight for the analysis of these systems is that the Lagrangian and Hamiltonian theory of classical mechanics applies to a probabilistic formalization of the problem, in the sense that the system's state in phase space follows a quasi-potential that is proportional to the solution of the Hamilton-Jacobi-Bellman equation.

The next section reviews several systems and methods in mathematical physics that underpin integrals of the motion and examples of the potential, in support of a discussion of the quasi-potential in Section 2.4.

2.2 Mathematical Physics Overview

We begin by analysing the invariants of both the frictionless and damped simple harmonic oscillator (SHO), which is governed by a second-order ODE. The relevance of second-order ODEs will be discussed more fully below, but originates from the Smoluchowski-Kramers approximation of Langevin's equation for Brownian motion [10], according to which the small mass of the Brownian particle justifies neglecting the highest derivative term. This leads to a diffusion equation which is analogous to the first-order systems of ODEs modelling metabolic pathways and which forms the basis of the quasi-potential formalism. Hence, we are hoping that analytical insight in the invariants of the damped SHO will help us in the analysis of dissipative metabolic systems.

2.2.1 First Integral of the Simple Harmonic Oscillator

The ODE governing the motion of the SHO is given by the following second-order differential equation, derivable from Newton's law:

$$\ddot{x} + \omega_0^2 x = 0, \tag{2.1}$$

where the dot ($\dot{}$) indicates differentiation with respect to time and $\omega_0 = \sqrt{k/m}$ is the natural frequency of oscillation, with k the spring constant and m the mass of the particle acted upon by the spring.

Although the solution of Eq. (2.1) is trivially obtainable as a complex exponential that leads to the trigonometric functions, it is instructive to follow Tabor's step-by-step integration [44]:

$$\begin{aligned}
m\ddot{x} + kx &= 0 \\
m\frac{d}{dt}(\dot{x}) + kx &= 0 \\
m\frac{d}{dx}(\dot{x})\frac{dx}{dt} + k\frac{d}{dx}\left(\frac{x^2}{2}\right) &= 0 \\
m\frac{dx}{dt}\frac{d}{dx}(\dot{x}) + k\frac{d}{dx}\left(\frac{x^2}{2}\right) &= 0 \\
m\dot{x}\frac{d}{dx}(\dot{x}) + k\frac{d}{dx}\left(\frac{x^2}{2}\right) &= 0 \\
m\frac{d}{dx}\left(\frac{\dot{x}^2}{2}\right) + k\frac{d}{dx}\left(\frac{x^2}{2}\right) &= 0 \\
\frac{d}{dx}\left[\frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2\right] &= 0 \\
\frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 &= \text{Const.} = E(x, \dot{x}). \qquad (2.2)
\end{aligned}$$

This is the archetypical integral of the motion, or 'first integral'. It is the total mechanical energy of the oscillator, i.e. the sum of its potential and kinetic energies, which is constant since there is no friction. It is a function of the phase space variables and does not depend explicitly on time. Eq. (2.2) can be rearranged, leading to a second integration and the familiar solution:

$$\begin{aligned}
\left(\frac{dx}{dt}\right)^2 &= \frac{2E}{m} - \frac{k}{m}x^2 \\
\frac{dx}{dt} &= \sqrt{\frac{2E}{m} - \frac{k}{m}x^2} \\
\frac{dx}{\sqrt{\frac{2E}{m} - \frac{k}{m}x^2}} &= dt \\
\frac{dx}{\sqrt{\frac{2E}{k} - x^2}} &= \sqrt{\frac{k}{m}}dt \\
-\cos^{-1}\left(\frac{x}{\sqrt{\frac{2E}{k}}}\right) &= \sqrt{\frac{k}{m}}t + \phi_0 \\
x(t) &= \sqrt{\frac{2E}{k}}\cos\left(\sqrt{\frac{k}{m}}t + \phi_0\right) = A\cos(\omega_0 t + \phi_0). \qquad (2.3)
\end{aligned}$$

2.2.2 First Integral of the Damped Simple Harmonic Oscillator

Since the damped SHO is also modelled by a linear and fully integrable ODE, we know that we can easily obtain its two constants of integration, which we might expect to be expressible as two constants of the motion. Surprisingly, however, the damped SHO also has a first integral, called 'Bohlin's integral' [20]. This is surprising because, since the damping causes the total energy to decrease, it is not immediately clear what physical property might be conserved.

Gettys et al. [20] discuss several constants and integrals of the damped SHO, only two of which can be independent. Since metabolic systems are also dissipative, it could be useful to understand in depth the invariants of the motion of the damped SHO. Gettys et al. [20] provide the expression for Bohlin's integral but do not derive it.[4] Interestingly, applying the same method used to find the energy integral for the SHO we were able to derive this result. We start by recalling the elementary solution of the ODE

$$\ddot{x} + 2\mu\dot{x} + \omega_0^2 x = 0, \tag{2.4}$$

where μ is the coefficient of friction per unit mass and the factor of 2 is just for algebraic convenience. The standard solution is expressed in terms of the eigenvalues of the characteristic equation, for the three cases overdamped, critically damped, and underdamped:

$$x(t) = A_1 e^{\alpha_1 t} + A_2 e^{\alpha_2 t}, \tag{2.5}$$

where $\alpha_{1,2}$ are the eigenvalues:

$$\alpha_{1,2} = \begin{cases} -\mu \pm \sqrt{\mu^2 - \omega_0^2} = -\mu \pm \zeta & \mu > \omega_0, \quad \text{overdamped} \\ -\mu & \mu = \omega_0, \quad \text{critically damped} \\ -\mu \pm i\sqrt{\omega_0^2 - \mu^2} = -\mu \pm i\omega & \mu < \omega_0, \quad \text{underdamped,} \end{cases} \tag{2.6}$$

where for convenience we have defined the new variables $\zeta = \sqrt{\mu^2 - \omega_0^2}$ and $\omega = \sqrt{\omega_0^2 - \mu^2}$. The repeated eigenvalue for the critically damped case leads to a slighty different form of the solution:

$$x(t) = A_1 e^{-\mu t} + A_2 t e^{-\mu t}. \tag{2.7}$$

The constants of integration $A_{1,2}$ are real for the overdamped and critically damped cases, and complex for the underdamped case. For the latter, they lead to the following real solution:

$$\begin{aligned}
x(t) &= (a + ib)e^{(-\mu + i\omega)t} + (a - ib)e^{(-\mu - i\omega)t} \\
&= e^{-\mu t}\left[(a + ib)e^{i\omega t} + (a - ib)e^{-i\omega t}\right] \\
&= e^{-\mu t}\left[\left(\frac{1}{2}Ce^{i\phi}\right)e^{i\omega t} + \left(\frac{1}{2}Ce^{-i\phi}\right)e^{-i\omega t}\right] \\
&= \frac{1}{4}Ce^{-\mu t}\left[2e^{i\omega t}e^{i\phi} + e^{-i\omega t}e^{-i\phi}\right] \\
&= \frac{1}{4}Ce^{-\mu t}\Big[e^{i\omega t}e^{i\phi} + e^{i\omega t}e^{-i\phi} + e^{-i\omega t}e^{i\phi} + e^{-i\omega t}e^{-i\phi} \\
&\qquad\qquad + e^{i\omega t}e^{i\phi} - e^{i\omega t}e^{-i\phi} - e^{-i\omega t}e^{i\phi} + e^{-i\omega t}e^{-i\phi}\Big] \\
&= \frac{1}{4}Ce^{-\mu t}\left[\left(e^{i\omega t} + e^{-i\omega t}\right)\left(e^{i\phi} + e^{-i\phi}\right) - i^2\left(e^{i\omega t} - e^{-i\omega t}\right)\left(e^{i\phi} - e^{-i\phi}\right)\right] \\
&= Ce^{-\mu t}\left[\frac{e^{i\omega t} + e^{-i\omega t}}{2}\frac{e^{i\phi} + e^{-i\phi}}{2} - \frac{e^{i\omega t} - e^{-i\omega t}}{2i}\frac{e^{i\phi} - e^{-i\phi}}{2i}\right] \\
&= Ce^{-\mu t}\left[\cos\omega t\cos\phi - \sin\omega t\sin\phi\right] \\
&= Ce^{-\mu t}\cos(\omega t + \phi),
\end{aligned} \tag{2.8}$$

where the constants $C = \sqrt{a^2 + b^2}$ and $\phi = \tan^{-1}(b/a)$ are real.

[4] Bohlin himself, in 1908, claimed that Euler had originally derived this integral, but Gettys et al. were not able to find this derivation [20].

Gettys et al. do not use the eigenvalues directly but two parameters that are similar:

$$\lambda_{1,2} = \begin{cases} \mu \pm \sqrt{\mu^2 - \omega_0^2} = \mu \pm \zeta & \mu > \omega_0, \quad \text{overdamped} \\ \mu & \mu = \omega_0, \quad \text{critically damped} \\ \mu \mp i\sqrt{\omega_0^2 - \mu^2} = \mu \mp i\omega & \mu < \omega_0, \quad \text{underdamped,} \end{cases} \tag{2.9}$$

and in terms of which the ODE becomes

$$\ddot{x} + (\lambda_1 + \lambda_2)\dot{x} + \lambda_1\lambda_2 x = 0. \tag{2.10}$$

This ODE is invariant under transposition of λ_1 and λ_2. Gettys et al. define $\lambda_{1,2} = \mu \pm \sqrt{\mu^2 - \omega_0^2}$ for the overdamped case and $\lambda_{1,2} = \mu \pm i\sqrt{\omega_0^2 - \mu^2}$ for the underdamped case but, as shown in Eq. (2.9), we found that to make the algebra work out opposite signs of the square-roots need to be used in the two cases. To see why the signs need to be treated differently in the overdamped and underdamped cases, first we state explicitly the definitions and their immediate consequences:

$$2\mu = \lambda_1 + \lambda_2 \tag{2.11}$$

$$\omega_0^2 = \lambda_1\lambda_2 \tag{2.12}$$

$$\begin{aligned} \zeta = \sqrt{\mu^2 - \omega_0^2} &= \sqrt{\left(\frac{\lambda_1 + \lambda_2}{2}\right)^2 - \lambda_1\lambda_2} = \sqrt{\frac{\lambda_1^2}{4} + \frac{\lambda_1\lambda_2}{2} + \frac{\lambda_2^2}{4} - \lambda_1\lambda_2} \\ &= \sqrt{\frac{\lambda_1^2}{4} - \frac{\lambda_1\lambda_2}{2} + \frac{\lambda_2^2}{4}} = \sqrt{\frac{1}{4}(\lambda_1^2 - 2\lambda_1\lambda_2 + \lambda_2^2)} \\ &= \frac{\lambda_1 - \lambda_2}{2} \end{aligned} \tag{2.13}$$

$$\begin{aligned} \omega = \sqrt{\omega_0^2 - \mu^2} &= \sqrt{\lambda_1\lambda_2 - \left(\frac{\lambda_1 + \lambda_2}{2}\right)^2} = \sqrt{\lambda_1\lambda_2 - \frac{\lambda_1^2}{4} - \frac{\lambda_1\lambda_2}{2} - \frac{\lambda_2^2}{4}} \\ &= \sqrt{-\frac{\lambda_1^2}{4} + \frac{\lambda_1\lambda_2}{2} - \frac{\lambda_2^2}{4}} = \sqrt{-\frac{1}{4}(\lambda_1^2 - 2\lambda_1\lambda_2 + \lambda_2^2)} \\ &= i\frac{\lambda_1 - \lambda_2}{2}. \end{aligned} \tag{2.14}$$

Now we compare the value of λ_1 for both cases and using both signs for the square-roots, showing that in each case one of the choices for the sign leads to an inconsistency:

$$\lambda_1 = \begin{cases} \mu + \zeta = \frac{\lambda_1+\lambda_2}{2} + \frac{\lambda_1-\lambda_2}{2} = \lambda_1 & \text{OK} \\ \mu - \zeta = \frac{\lambda_1+\lambda_2}{2} - \frac{\lambda_1-\lambda_2}{2} = \lambda_2 & \text{Contradiction} \\ \mu + i\omega = \frac{\lambda_1+\lambda_2}{2} + i\left(i\frac{\lambda_1-\lambda_2}{2}\right) = \frac{\lambda_1+\lambda_2}{2} - \frac{\lambda_1-\lambda_2}{2} = \lambda_2 & \text{Contradiction} \\ \mu - i\omega = \frac{\lambda_1+\lambda_2}{2} - i\left(i\frac{\lambda_1-\lambda_2}{2}\right) = \frac{\lambda_1+\lambda_2}{2} + \frac{\lambda_1-\lambda_2}{2} = \lambda_1 & \text{OK.} \end{cases} \tag{2.15}$$

And the converse applies to λ_2. Figure 2.1 provides a visualization of these parameters. As a consequence of these definitions, we have that

$$\begin{array}{cc} \text{Overdamped} & \text{Underdamped} \\ \lambda_1 = -\alpha_2 & \lambda_1 = -\alpha_1 \\ \lambda_2 = -\alpha_1 & \lambda_2 = -\alpha_2. \end{array} \tag{2.16}$$

To derive Bohlin's integral, we integrate Eq. (2.4) step-by-step:

$$\frac{d}{dt}(\dot{x}) + 2\mu\frac{dx}{dt} + \omega_0^2\frac{d}{dx}\left(\frac{x^2}{2}\right) = 0$$

$$\frac{d}{dx}\left(\frac{dx}{dt}\right)\frac{dx}{dt} + 2\mu\frac{dx}{dx}\frac{dx}{dt} + \omega_0^2 x = 0$$

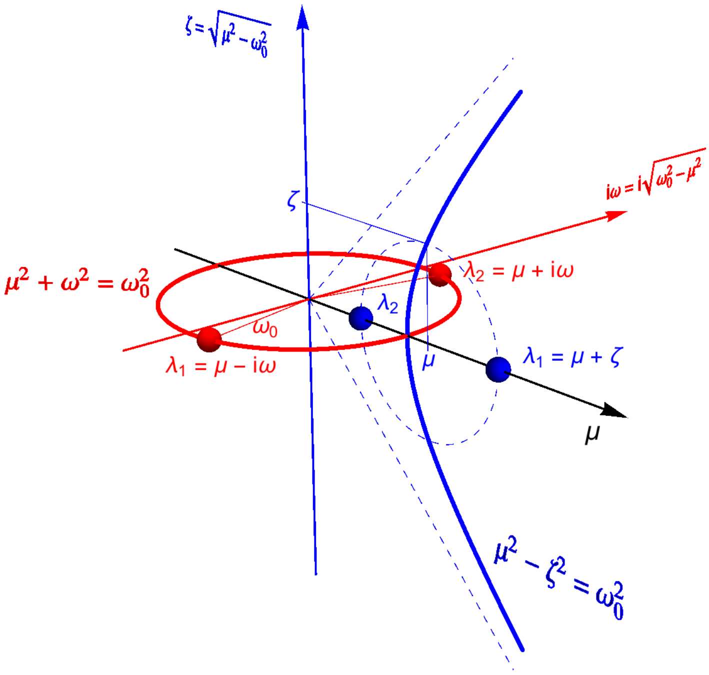

Fig. 2.1: **Eigenvalue-like parameters from [20] for the damped simple harmonic oscillator**

$$\begin{aligned}
\frac{dx}{dt}\frac{d}{dx}\left(\frac{dx}{dt}\right) + 2\mu\frac{dx}{dt}\frac{dx}{dx} + \omega_0^2 x &= 0 \\
v\frac{dv}{dx} + 2\mu v\frac{dx}{dx} + \omega_0^2 x &= 0 \\
v\frac{d}{dx}(v + 2\mu x) + \omega_0^2 x &= 0 \\
\frac{d}{dx}(v + 2\mu x) &= -\omega_0^2\frac{x}{v} \\
\frac{dv}{dx} &= -2\mu - \omega_0^2\frac{x}{v},
\end{aligned} \tag{2.17}$$

where $v = \dot{x} = \frac{dx}{dt}$. Now we introduce the new variable $z = v/x$, such that $\frac{dv}{dx} = z + x\frac{dz}{dx}$. Substituting in (2.17),

$$\begin{aligned}
z + x\frac{dz}{dx} &= -2\mu - \omega_0^2\frac{1}{z} \\
x\frac{dz}{dx} &= -z - 2\mu - \omega_0^2\frac{1}{z} \\
x\frac{dz}{dx} &= -\frac{z^2 + 2\mu z + \omega_0^2}{z} \\
\frac{zdz}{z^2 + 2\mu z + \omega_0^2} &= -\frac{dx}{x}
\end{aligned}$$

$$-\frac{\mu}{\sqrt{\omega_0^2 - \mu^2}}\tan^{-1}\left[\frac{z + \mu}{\sqrt{\omega_0^2 - \mu^2}}\right] + \frac{1}{2}\log(z^2 + 2\mu z + \omega_0^2) = \log\frac{1}{x} + C_1. \tag{2.18}$$

Rearranging,

$$\begin{aligned}
C_1 &= \log(z^2 + 2\mu z + \omega_0^2)^{1/2} + \log x - \frac{\mu}{\sqrt{\omega_0^2 - \mu^2}}\tan^{-1}\left[\frac{z + \mu}{\sqrt{\omega_0^2 - \mu^2}}\right] \\
&= \log\left[x\sqrt{\left(\frac{v}{x}\right)^2 + 2\mu\left(\frac{v}{x}\right) + \omega_0^2}\right] - \frac{\mu}{\sqrt{\omega_0^2 - \mu^2}}\tan^{-1}\left[\frac{v/x + \mu}{\sqrt{\omega_0^2 - \mu^2}}\right] \\
&= \frac{1}{2}\log(v^2 + 2\mu v x + \omega_0^2 x^2) - \frac{\mu}{\sqrt{\omega_0^2 - \mu^2}}\tan^{-1}\left[\frac{v + \mu x}{x\sqrt{\omega_0^2 - \mu^2}}\right].
\end{aligned} \tag{2.19}$$

Using the identity

$$\tan^{-1}(y) = \frac{1}{2}i[\log(1 - iy) - \log(1 + iy)], \tag{2.20}$$

the corresponding factor in (2.19) becomes

$$\begin{aligned}
\tan^{-1}\left[\frac{v+\mu x}{x\sqrt{\omega_0^2-\mu^2}}\right] &= \frac{1}{2}i\left[\log\left(1 - i\frac{v+\mu x}{x\sqrt{\omega_0^2-\mu^2}}\right) - \log\left(1 + i\frac{v+\mu x}{x\sqrt{\omega_0^2-\mu^2}}\right)\right] \\
&= \frac{1}{2}i\log\left[\frac{x\sqrt{\omega_0^2-\mu^2} - i(v+\mu x)}{x\sqrt{\omega_0^2-\mu^2} + i(v+\mu x)}\right] \\
&= \frac{1}{2}i\log\left[\frac{x\frac{i}{2}(\lambda_1-\lambda_2) - iv - \frac{i}{2}(\lambda_1+\lambda_2)x)}{x\frac{i}{2}(\lambda_1-\lambda_2) + iv + \frac{i}{2}(\lambda_1+\lambda_2)x)}\right] \\
&= \frac{1}{2}i\log\left[\frac{-i(v+\lambda_2 x)}{i(v+\lambda_1 x)}\right] = \frac{1}{2}i\log\left[-\frac{(v+\lambda_2 x)}{(v+\lambda_1 x)}\right].
\end{aligned} \tag{2.21}$$

Plugging this into (2.19) and expressing everything in terms of the λ parameters,

$$\begin{aligned}
C_1 &= \frac{1}{2}\log(v^2 + 2\mu vx + \omega_0^2 x^2) - \frac{\mu}{\sqrt{\omega_0^2-\mu^2}}\left(\frac{1}{2}i\log\left[-\frac{(v+\lambda_2 x)}{(v+\lambda_1 x)}\right]\right) \\
&= \frac{1}{2}\log\left[v^2 + (\lambda_1+\lambda_2)vx + \lambda_1\lambda_2 x^2\right] + i\frac{\lambda_1+\lambda_2}{\lambda_1-\lambda_2}\left(\frac{1}{2}i\log\left[-\frac{(v+\lambda_2 x)}{(v+\lambda_1 x)}\right]\right) \\
&= \frac{1}{2}\log\left[(v+\lambda_1 x)(v+\lambda_2 x)\right] - \frac{1}{2}\frac{\lambda_1+\lambda_2}{\lambda_1-\lambda_2}\log\left[-\frac{v+\lambda_2 x}{v+\lambda_1 x}\right] \\
&= \log\left[(v+\lambda_1 x)(v+\lambda_2 x)\right]^{\frac{1}{2}} + \log\left[\left(-\frac{v+\lambda_2 x}{v+\lambda_1 x}\right)^{-\frac{\lambda_1+\lambda_2}{\lambda_1-\lambda_2}}\right]^{\frac{1}{2}} \\
&= \log\left[(v+\lambda_1 x)(v+\lambda_2 x)\right]^{\frac{1}{2}} + \log\left[\left(-\frac{v+\lambda_1 x}{v+\lambda_2 x}\right)^{\frac{\lambda_1+\lambda_2}{\lambda_1-\lambda_2}}\right]^{\frac{1}{2}} \\
&= \log\left[(v+\lambda_1 x)(v+\lambda_2 x)\left(-\frac{v+\lambda_1 x}{v+\lambda_2 x}\right)^{\frac{\lambda_1+\lambda_2}{\lambda_1-\lambda_2}}\right]^{\frac{1}{2}}.
\end{aligned}$$

With a few more steps, we get

$$\begin{aligned}
(-1)^{\frac{\lambda_1+\lambda_2}{\lambda_1-\lambda_2}}(e^{C_1})^2 &= (v+\lambda_1 x)^{1+\frac{\lambda_1+\lambda_2}{\lambda_1-\lambda_2}}(v+\lambda_2 x)^{1-\frac{\lambda_1+\lambda_2}{\lambda_1-\lambda_2}} \\
C_2 &= (v+\lambda_1 x)^{\frac{2\lambda_1}{\lambda_1-\lambda_2}}(v+\lambda_2 x)^{\frac{-2\lambda_2}{\lambda_1-\lambda_2}} \\
C_2 &= \frac{(v+\lambda_1 x)^{\frac{2\lambda_1}{\lambda_1-\lambda_2}}}{(v+\lambda_2 x)^{\frac{2\lambda_2}{\lambda_1-\lambda_2}}} \\
(C_2)^{\frac{\lambda_1-\lambda_2}{2\lambda_2}} &= \frac{(v+\lambda_1 x)^{\lambda_1}}{(v+\lambda_2 x)^{\lambda_2}} \\
B &= \frac{(v+\lambda_1 x)^{\lambda_1}}{(v+\lambda_2 x)^{\lambda_2}},
\end{aligned} \tag{2.22}$$

where in general C_1, C_2 and B are complex constants. When the system is critically damped $B = 1$, so we will not discuss it further. C_2 involves a negative 1 raised to a real number for the overdamped case, which is not allowed, and to an imaginary number for the underdamped case, which is meaningless because its expression in complex polar notation would involve the logarithm of a negative number:

$$\frac{\lambda_1+\lambda_2}{\lambda_1-\lambda_2} = \begin{cases} \frac{\mu}{\zeta} & \text{Overdamped} \\ i\frac{\mu}{\omega} & \text{Underdamped.} \end{cases} \tag{2.23}$$

It is not clear how this issue can be resolved. Assuming that 'complex constant' is sufficient, this first integral is valid for all absolute and relative values of μ and ω_0, i.e. for all levels of damping.

We can visualize the solution trajectories in phase space as level sets of Bolhin's integral. When the system is overdamped B is real, whereas when it is underdamped B is complex. In order to visualize this function let us find other ways to express it. To verify the expression for Bohlin's integral we substitute Eqs. (2.5) and (2.16) into (2.22):

Overdamped

$$\frac{\left[\alpha_1 A_1 e^{\alpha_1 t}+\alpha_2 A_2 e^{\alpha_2 t}-\alpha_2 A_1 e^{\alpha_1 t}-\alpha_2 A_2 e^{\alpha_2 t}\right]^{-\alpha_2}}{\left[\alpha_1 A_1 e^{\alpha_1 t}+\alpha_2 A_2 e^{\alpha_2 t}-\alpha_1 A_1 e^{\alpha_1 t}-\alpha_1 A_2 e^{\alpha_2 t}\right]^{-\alpha_1}}$$

$$\frac{\left[A_1(\alpha_1-\alpha_2)e^{\alpha_1 t}\right]^{-\alpha_2}}{\left[A_2(\alpha_2-\alpha_1)e^{\alpha_2 t}\right]^{-\alpha_1}}$$

$$\frac{A_2^{\alpha_1}\left(\alpha_2-\alpha_1\right)^{\alpha_1}}{A_1^{\alpha_2}\left(\alpha_1-\alpha_2\right)^{\alpha_2}}$$

$$\frac{A_2^{-\mu+\zeta}}{A_1^{-\mu-\zeta}}\frac{\left[-\mu-\zeta-(-\mu+\zeta)\right]^{-\mu+\zeta}}{\left[-\mu+\zeta-(-\mu-\zeta)\right]^{-\mu-\zeta}}$$

$$\frac{A_2^{-\mu+\zeta}}{A_1^{-\mu-\zeta}}\frac{\left(-2\zeta\right)^{-\mu+\zeta}}{\left(2\zeta\right)^{-\mu-\zeta}}$$

$$\frac{(-A_2)^{-\mu+\zeta}}{A_1^{-\mu-\zeta}}\left(2\zeta\right)^{-\mu+\zeta+\mu+\zeta}$$

$$\boxed{\frac{(-A_2)^{-\mu+\zeta}}{A_1^{-\mu-\zeta}}\left(2\zeta\right)^{2\zeta}}$$

Underdamped

$$\frac{\left[\alpha_1 A_1 e^{\alpha_1 t}+\alpha_2 A_2 e^{\alpha_2 t}-\alpha_1 A_1 e^{\alpha_1 t}-\alpha_1 A_2 e^{\alpha_2 t}\right]^{-\alpha_1}}{\left[\alpha_1 A_1 e^{\alpha_1 t}+\alpha_2 A_2 e^{\alpha_2 t}-\alpha_1 A_1 e^{\alpha_1 t}-\alpha_1 A_2 e^{\alpha_2 t}\right]^{-\alpha_2}}$$

$$\frac{\left[A_2(\alpha_2-\alpha_1)e^{\alpha_2 t}\right]^{-\alpha_1}}{\left[A_1(\alpha_1-\alpha_2)e^{\alpha_1 t}\right]^{-\alpha_2}}$$

$$\frac{A_1^{\alpha_2}\left(\alpha_1-\alpha_2\right)^{\alpha_2}}{A_2^{\alpha_1}\left(\alpha_2-\alpha_1\right)^{\alpha_1}} \tag{2.24}$$

$$\frac{A_1^{-\mu-i\omega}}{A_2^{-\mu+i\omega}}\frac{\left[-\mu+i\omega-(-\mu-i\omega)\right]^{-\mu-i\omega}}{\left[-\mu-i\omega-(-\mu+i\omega)\right]^{-\mu+i\omega}}$$

$$\frac{(a+ib)^{-\mu-i\omega}}{(a-ib)^{-\mu+i\omega}}\frac{(2i\omega)^{-\mu-i\omega}}{(-2i\omega)^{-\mu+i\omega}}$$

$$\frac{(a+ib)^{-2\mu}}{(a^2+b^2)^{-\mu+i\omega}}\frac{\left(2\omega e^{i\frac{\pi}{2}}\right)^{-\mu-i\omega}}{\left(2\omega e^{-i\frac{\pi}{2}}\right)^{-\mu+i\omega}}$$

$$\frac{(a^2+b^2)^{-\mu}e^{-2i\mu\tan^{-1}\left(\frac{b}{a}\right)}}{(a^2+b^2)^{-\mu+i\omega}}\frac{(2\omega)^{-\mu-i\omega}\ e^{\frac{\omega\pi}{2}-i\frac{\mu\pi}{2}}}{(2\omega)^{-\mu+i\omega}\ e^{\frac{\omega\pi}{2}+i\frac{\mu\pi}{2}}}$$

$$\left(a^2+b^2\right)^{-i\omega}e^{-2i\mu\tan^{-1}\left(\frac{b}{a}\right)}\ \left(2\omega\right)^{-2i\omega}e^{-i\mu\pi}$$

$$\boxed{e^{-i\left[\omega\log(a^2+b^2)+2\mu\tan^{-1}\left(\frac{b}{a}\right)+\mu\pi+(2\omega)\log(2\omega)\right]}}$$

The undetermined constants in the boxed expressions for B are found by setting (2.5) and its derivative equal to the initial conditions,

$$x(0)=A_1+A_2=x_0 \tag{2.25}$$

$$\dot{x}(0)=\alpha_1 A_1+\alpha_2 A_2=v_0, \tag{2.26}$$

leading to

Overdamped

$$A_1=\frac{v_0+(\mu+\zeta)x_0}{2\zeta}=\frac{v_0+\lambda_1 x_0}{\lambda_1-\lambda_2}$$

$$A_2=-\frac{v_0+(\mu-\zeta)x_0}{2\zeta}=-\frac{v_0+\lambda_2 x_0}{\lambda_1-\lambda_2}$$

Underdamped

$$a=\frac{x_0}{2} \tag{2.27}$$

$$b=-\frac{v_0+\mu x_0}{2\omega}=i\frac{v_0+\frac{\lambda_1+\lambda_2}{2}x_0}{\lambda_1-\lambda_2}. \tag{2.28}$$

As expected, plugging these expressions into the boxed equations above recovers the expression for Bohlin's integral, Eq. (2.22), in terms of the initial values x_0 and v_0, which confirms the fact that it

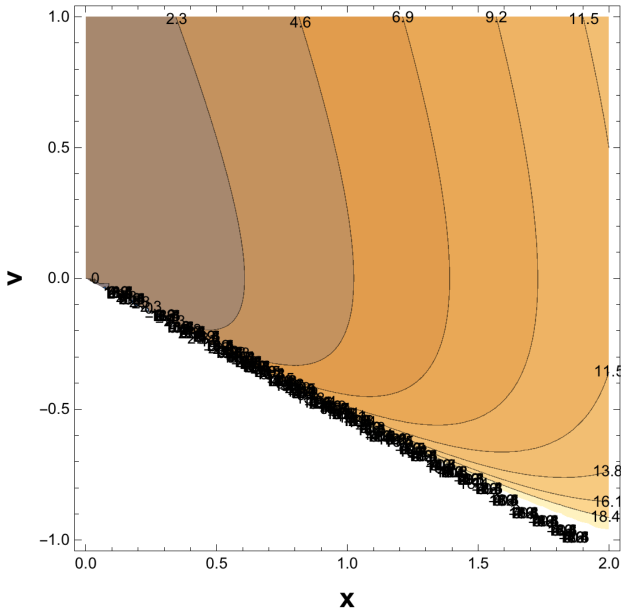

Fig. 2.2: **Level sets of Bohlin's integral in phase space for $\omega_0 = 1$ and $\mu = 1.2$**

is constant. The level sets of Bohlin's integral are shown for the overdamped case in Figure 2.2. The curves shown correspond to actual solution trajectories in phase space (see e.g. [45]).

For the complex, underdamped case the solution trajectories are spirals into the origin. It is possible to visualize them directly as the level sets of a complex-valued B function because when expressed in polar form its modulus is 1, so its level sets correspond to constant real values of its argument:

$$B = e^{-i\left[\sqrt{\omega_0^2-\mu^2}\log(v_0^2+2\mu v_0 x_0+\mu^2 x_0^2)+2\mu\tan^{-1}\left(\frac{x_0\sqrt{\omega_0^2-\mu^2}}{v_0+\mu x_0}\right)\right]}. \tag{2.29}$$

For $\omega_0 = 1$ and $\mu = 0.9$, Figure 2.2 shows these trajectories, with some singular behaviour along the negative diagonal.

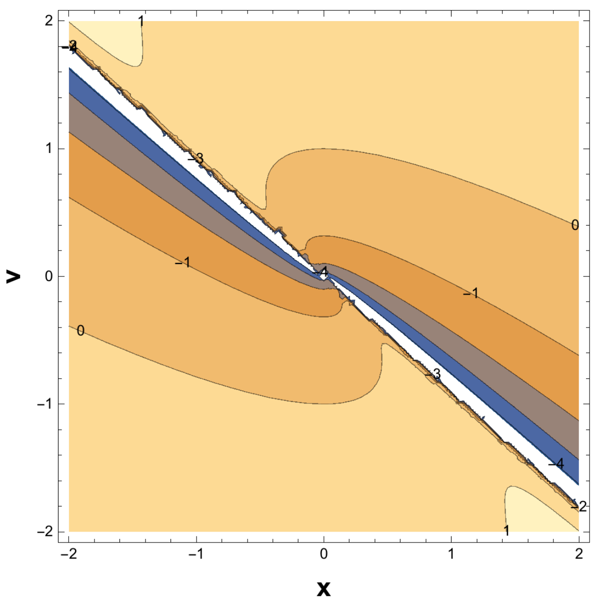

Fig. 2.3: **Level sets of Bohlin's integral in phase space for $\omega_0 = 1$ and $\mu = 0.9$**

We can also generate a more abstract diagram in order to visualize individual values of B, both real and complex, for different damping conditions. To simplify the calculation we set $v_0 = 0$, $x_0 = 1$, and $\omega_0 = 1$. Thus, the only variable left is the damping coefficient μ:

$$B(\mu) = \frac{\lambda_1^{\lambda_1}}{\lambda_2^{\lambda_2}} \begin{cases} \frac{\left(\mu+\zeta\right)^{\mu+\zeta}}{\left(\mu-\zeta\right)^{\mu-\zeta}} = \frac{\left(\mu+\sqrt{\mu^2-1}\right)^{\mu+\sqrt{\mu^2-1}}}{\left(\mu-\sqrt{\mu^2-1}\right)^{\mu-\sqrt{\mu^2-1}}}, & \text{Overdamped} \\ \\ \frac{\left(\mu-i\omega\right)^{\mu-i\omega}}{\left(\mu+i\omega\right)^{\mu+i\omega}} = \frac{\left(\mu-i\sqrt{1-\mu^2}\right)^{\mu-i\sqrt{1-\mu^2}}}{\left(\mu+i\sqrt{1-\mu^2}\right)^{\mu+i\sqrt{1-\mu^2}}} = e^{i2\mu\tan^{-1}\left(-\frac{\sqrt{1-\mu^2}}{\mu}\right)}, & \text{Underdamped} \end{cases} \tag{2.30}$$

As μ is decreased towards 0 the system will be overdamped until $\mu = 1$, and underdamped thereafter. Figure 2.4 shows this progression in a 3-D diagram that is similar to Figure 2.1: the vertical μ-B plane is Real and corresponds to the overdamped case, whereas the horizontal μ-ω plane is complex. The μ-axis doubles up also as the real part of B. Similarly, the ω-axis doubles up also as the imaginary part of B.

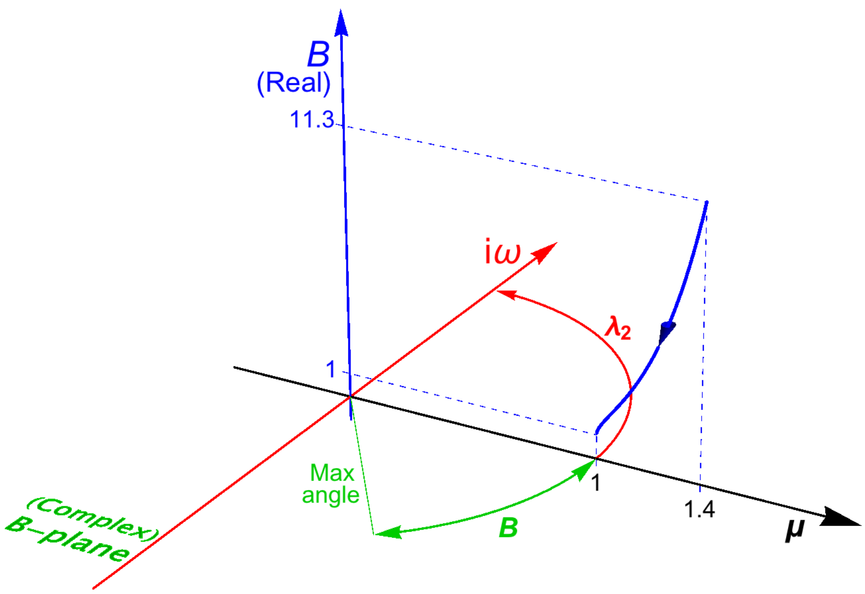

Fig. 2.4: **Real and complex values of Bohlin's integral for $\omega_0 = 1$ and different damping**

The thick blue curve is the graph of Eq. (2.30)a. The value of B starts fairly high at 11.3 when $\mu = 1.4$ and decreases towards 1 as μ approaches 1 from above. At $\mu = 1$ the value of B becomes complex and is shown as the green circular arc of modulus 1, which is the graph of Eq. (2.30)b. The complex visualization is harder to interpret and requires more explanation.

Eq. (2.30)b is, technically, a complex function of two complex variables, λ_1 and λ_2. However, since they are conjugates of each other, we can use just one of them for purposes of visualization, and chose λ_2. This makes $B(\lambda_2)$ a normal complex function of a complex variable, which is usually visualized as a mapping from the plane to the plane. The red circular arc in the first quadrant, therefore, represents the locus of complex values taken on by λ_2 as μ goes from 1 towards 0. The values of B that correspond to this locus are shown as the green circular arc in the fourth quadrant. The arc is double-headed because the value of B, which equals 1 when $\mu = 1$, moves clockwise along the green arc as λ_2 moves counterclockwise along the red arc, reaches a maximum (negative) angle as shown in the figure that is approximately 0.92 radians, and then moves back towards 1 as λ_2 approaches i, the undamped limiting case. The maximum angle was found by taking the derivative of the argument of Eq. (2.30)b and setting it equal to zero, which led to the following equation

$$\tan^{-1}\left(-\frac{\sqrt{1-\mu^2}}{\mu}\right) = -\frac{\mu}{\sqrt{1-\mu^2}}, \tag{2.31}$$

whose root in the unit interval was found numerically as $\mu_{max} = 0.86$, $\theta_{max} = 52.78$ deg.[5]

The significance of the different values of B for different damping is unclear. The existence of this first integral appears to be related to the existence of eigenvalues for this problem, i.e. to its linear nature, since B's λ parameters are closely related to the eigenvalues. This property is likely to be relevant in higher dimensions, so we would expect similar first integrals to exist also for systems of two or more *linearly* coupled oscillators, e.g. as are discussed in Chapter 5.

Similarly, the fact that B goes from Real to Complex as the damping crosses $\mu = 1$ from above is not likely to signify anything other than a reflection of the field to which the solution itself belongs. It may be that higher real B values correspond to a faster shrinking of the phase volume, which would correspond to greater energy dissipation due to damping.

The details of the derivation and the functional forms of B were included here because as far as we know they have not been reported elsewhere[6] and could be interesting for further brainstorming about this simple system to investigate this and similar questions. However, although the concepts presented are helpful as a limiting case and as an example of a first integral, we can stop here since the problems we are interested in are non-linear and nothing like eigenvalues is likely to be relevant to the properties of their solutions. Accordingly, we now turn to a rather more complex 2nd-order system, which helps introduce the relevance of the potential, and of a time-dependent potential in particular, for characterizing the behaviour of dynamical systems.

2.2.3 Non-Linear Coupling and the Time-Dependent Effective Potential

An example of a time-dependent potential surface that has served as one of the inspirations for the concept of dynamical stability can be derived for the non-linear turntable oscillator [12]. This oscillator, shown in Figure 2.5, is a model of the cross-section of a vertical thin elastic beam fixed at its base and free to bend and twist at its top. Thus, the beam can be seen as a stack of such turntables. The spring k_1 models the twisting return force, k_2 the bending return force, with J and m the corresponding inertias.[7] The turntable has radius R (not drawn), it rotates frictionlessly about a central pivot (also not shown), and as the cross-section of a vertical beam it rotates in a horizontal plane, so gravity plays no part.

The figure also shows the generalized Lagrangian coordinates s and θ, each measured from the neutral position of its respective spring. Using dimensional analysis (e.g. [35]), the governing Lagrangian equations of motion can be rendered dimensionless as

$$\ddot{\theta}(1+s^2) + 2s\dot{s}\dot{\theta} + \theta = 0 \tag{2.32}$$

$$\ddot{s} + (P - \dot{\theta}^2)s = 0, \tag{2.33}$$

where

$$\theta \text{ (already dimensionless)}, \qquad s = r/R, \qquad P = \frac{J/mR^2}{k_1/k_2}, \tag{2.34}$$

[5] The 'max' subscript only refers to the maximum absolute value of θ, clearly not of μ since that's decreasing down to zero. So in the case of μ it means 'the value of μ that maximizes $|\theta|$'. The same value corresponds to the *minimum* value of the real part of B.

[6] A brief mention of this integral is also made by Whittaker [49, p. 163].

[7] Rotational moment of inertia and linear inertia, respectively.

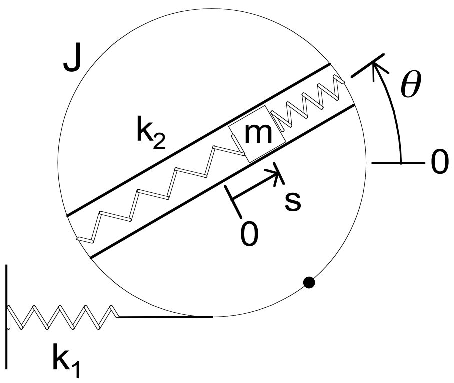

Fig. 2.5: **Non-linear turntable oscillator** [12]

and r is the radial coordinate from the centre of the turntable. The factor $(1+s^2)$ in Eq. (2.32) stands for a variable moment of rotational of inertia, due to the presence of mass m of variable radial location. The second term in Eq. (2.32) is the Coriolis force, and the $\dot{\theta}^2$ term in Eq. (2.33) is the centrifugal force (since the generalized coordinate s is defined in a rotating reference frame). As we would expect, the negative sign in front of $\dot{\theta}^2$ acts to decrease the effective spring constant (for a positive displacement s), and therefore also the frequency of oscillation.

We can now define a more abstract system whose state is in the configuration space $\mathbb{R}^2$ of the generalized coordinates and is therefore given by the ordered pair (θ, s). The force acting on such a system is a vector and, since the system is conservative, it can be expressed as the negative gradient of a potential function $U(\theta, s)$ that is analogous to the 'effective potential' of orbital classical mechanics (see e.g. [45]).

The idea of using the effective potential was originally inspired by Huygens's isochronous pendulum, whose motion can also be obtained by letting a small mass slide frictionlessly in a trough in the shape of a cycloid. Under these conditions, the component of the mass's weight-force tangent to the trough increases *linearly* with distance along the trough away from the minimum equilibrium point. As a consequence, the motion of such an oscillator (measured along the curvilinear cycloidal coordinate) behaves like a simple harmonic oscillator (SHO), whose frequency is independent of amplitude – hence the appellative 'isochronous'. The same set-up but using a parabolic trough, on the other hand, would exhibit the behaviour of a SHO only in its projection onto the x-plane. This is in fact the relationship between the position of a spring-mass system and its potential that we are exploring here.

Rewriting the governing equations of the turntable in the form of Newton's 2nd Law (time rate of change of momentum equals the net force), we obtain

$$\frac{d}{dt}[\dot{\theta}(1+s^2)] = -\theta \qquad = -\frac{\partial U}{\partial \theta} \tag{2.35}$$

$$\frac{d}{dt}[\dot{s}] = -(P-\dot{\theta}^2)s \qquad = -\frac{\partial U}{\partial s}. \tag{2.36}$$

Ignoring completely the left-hand side (LHS), straightforward integration yields

$$U(\theta, s) = \frac{1}{2}\theta^2 + \frac{1}{2}s^2(P-\dot{\theta}^2). \tag{2.37}$$

This is a time-dependent potential in the form of a paraboloid. Clearly, the full definition of this function requires knowledge of $\dot{\theta}(t)$ and, therefore, of the analytical solution. This oscillator is a non-integrable,[8] strongly non-linear, and in fact chaotic system, so no general solution is available analytically. However, the function $U(\theta, s)$ is still useful for gaining insight into this system and in

[8] 'Non-integrable' is meant in the loose physics sense, such that, even if we could find the Lie group for this system, it is very unlikely that we could then express its solution in terms of elementary functions.

particular into its stability properties. In fact, we can see that although the dependence of U on θ is static and a simple quadratic, the curvature of the parabola in the s-direction is time-dependent and can also switch sign. In other words, this paraboloid oscillates between a normal paraboloid and a hyperbolic paraboloid, as the value of $\dot{\theta}^2$ increases beyond the (constant) value of P.

Figure 2.6 shows two snapshots of this surface at two different times. The θ and s axes are not shown, but can be inferred from the shape of the surface: since it does not change along the θ axis, this can be seen as being oriented in the left-right direction. The s axis, therefore, is into and out of the paper. The state of the system is depicted as a red mass sliding on this surface. Since the effective potential of this oscillator is parabolic and not cycloidal, this visualization does not correspond exactly to the motion of a mass under the action of gravity sliding on a frictionless surface of this shape, but is merely meant to be a suggestive aid to intuition. Furthermore, whereas the angular coordinate θ is treated as a linear coordinate in Eq. (2.37) and therefore in drawing the surface in Figure 2.6, the top view of the trajectory of the ball, shown as the black curve, corresponds exactly to the path followed by the slider in the horizontal plane – meaning that in drawing the trajectory θ is used as a polar coordinate. This introduces an additional mismatch between the original idea of the cycloidal trough and the visualization. In spite of these limitations, the motion of the ball under the action of gravity on this "flapping" surface is helpful for visualizing what we mean by dynamical stability.

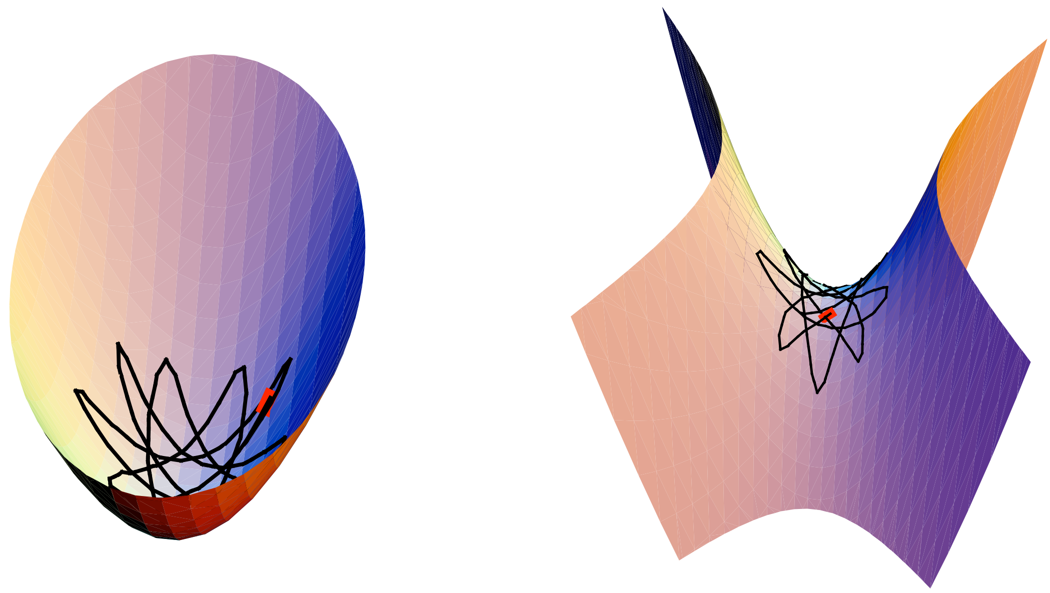

Fig. 2.6: **Two snapshots of the effective potential of the turntable oscillator**

The important point is that for the conditions corresponding to the case shown the system's (free) response is somewhere between periodic and chaotic. Thus, the "flapping" is close to but not quite periodic, and the trajectory of the "ball" does not retrace itself. In the language of KAM theory [2], the solution trajectory is (appears to be) quasi-periodic and, therefore, lies on a two-dimensional torus embedded in a four-dimensional phase space,[9] covering the whole surface of the torus as $t \to \infty$ and without retracing any of the points it touches (due to uniqueness). Nonetheless, it is clearly confined to a finite region of phase space (a consequence of the finite – and, in fact, invariant – total mechanical energy of this Hamiltonian system) and, further, it has a recognizable star-like shape. The fact that

[9] Defined by the coordinates $(\theta, \dot{\theta}, s, \dot{s})$.

for the case shown this system has a fairly stable and approximately predictable behaviour was the initial inspiration for the concept of 'dynamical stability'.

A much simpler analogous phenomenon from electrodynamics is known as a 'Paul trap' [41], an oscillating quadrupole. The significance of this phenomenon is that a charged test particle placed in a static electric field defined by point charges will always escape to infinity: there are no stable points on such a surface, no matter what the distribution of the charges that define it might be.[10] The only way to hold it in place is to make the potential time-dependent. Therefore, it appears that the concept of a time-dependent potential may be fundamentally important for achieving 'dynamical stability'. A similar observation applies to engineering systems that utilize active feedback control such as, for example, fighter jets: they are designed to be unstable in order to be able to respond extremely quickly to the pilot's commands, and are kept in check by active negative feedbacks.

Our contention, therefore, is that cell metabolism is able to respond quickly and appropriately to a wide range of time-dependent inputs and environmental conditions through some similar "active control" capability. It is therefore highly interesting that, as will be discussed below, the generalization of Hamilton-Jacobi theory that appears to be required to make further progress towards the BIOMICS objectives was a direct outgrowth of Richard Bellman's dynamic programming, whose most famous area of application has been the theory of optimal control.

2.2.4 Hamilton-Jacobi Theory and the Principle of Optimality

The research thread leading to this chapter started when we realized that the concept of the effective potential of dynamical systems as described above could be related to the quasi-potential developed by Freidlin and Wentzell [18], which we discovered in the more recent work of Zhou et al. [51]. In these references, the quasi-potential is defined as a solution to the Hamilton-Jacobi-Bellman equation. Thus, to understand its derivation we need to summarize briefly this well-established area of classical mechanics [45, 2] and of control theory [1], and in particular of dynamic programming [3, 4, 5].

2.2.4.1 Lagrangian Formulation

In standard treatments of analytical dynamics [45], the point is made that the Lagrangian formulation of mechanics is analogous to the Hamiltonian formulation, which is however more general and more desirable since it leads directly to quantum mechanics. The appeal of this theory (meaning analytical mechanics, i.e. both the Lagrangian and Hamiltonian formulations) is that it relies on the very general principle of least action, known as Hamilton's Principle, which is based on the Lagrangian function $L\colon \mathbb{R}^{2n+1} \to \mathbb{R}$:

$$L(q, \dot{q}, t) = T - U, \tag{2.38}$$

where $q(t)$ is the vector of dependent variables $q\colon \mathbb{R} \to \mathbb{R}^n$ known as 'generalized coordinates', which are functions of time, $\dot{q}(t)$ is the vector of their time derivatives, or velocities, $T(q, \dot{q})$ is the kinetic energy of the system, $U(q, \dot{q}, t)$ is the potential energy, and n is the number of generalized coordinates or 'degrees of freedom'. As shown, in general L and U can be functions of time. In this brief summary we will assume frictionless or 'Hamiltonian' systems.

The Lagrangian formulation of mechanics is appealing because it states that the behaviour of (most if not all) physical systems corresponds to a function $q(t)$ that minimizes the action functional:[11]

$$S = \int_{t_1}^{t_2} L(q, \dot{q}, t)\, dt. \tag{2.39}$$

[10] This is a consequence of the electric field being the negative gradient of a potential. Since by Gauss's law a gradient field is divergenceless, the potential satisfies Laplace's equation and is therefore a harmonic function. As such, its maxima and minima always lie on the boundary of the domain however it is defined.

[11] A 'functional' is a function of functions, in this case involving also an integral.

In the calculus of variations notation this is stated as

$$\delta \int_{t_1}^{t_2} L(q, \dot{q}, t)\, dt = 0, \tag{2.40}$$

where δ means 'variation in'. This condition is known as Hamilton's Principle and is a generalization of the zero-derivative condition of maximality or minimality of elementary calculus. In other words, the Lagrangian formulation is appealing because it shows that physical behaviour results from a global minimization principle. In fact, using the calculus of variations one can easily prove that the function $q(t)$ that minimizes the action must satisfy the n Euler-Lagrange differential equations:

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0, \tag{2.41}$$

where the subscript $i = \{1, \cdots, n\}$ indicates the independent component of q, i.e. the generalized coordinate, whose behaviour is governed by the corresponding equation. Most of the governing equations of mathematical physics in both classical and quantum mechanics (Newton's law, the wave equation, the heat equation, Schrödinger's equation, ...) are none other than the Euler-Lagrange equations instantiated in the different physical contexts.

2.2.4.2 Legendre Transform

The Hamiltonian formulation is derived by performing a Legendre transformation of the Lagrangian. The Legendre transformation transforms a function on a vector space to a function on the dual space [2]. The function in question is the Lagrangian, and it is transformed to the Hamiltonian. The source vector space is the space defined by the velocity vectors $\dot{q}$ at a point in configuration space (known generally as the Tangent Manifold at q, or TM_q) and the dual vector space TM_q^* is the space of the momentum vectors p. In classical mechanics these two spaces are coincident and both of dimension n.

To explain the Legendre transform let us take a convex function $f(x), f\colon \mathbb{R} \to \mathbb{R}$, i.e. such that $f''(x) > 0,\ \forall x$. Assume further that $f(0) = 0$. Although this assumption may be unnecessary it makes it easier to follow the derivation. In other words, we can imagine $f(x)$ to be a simple parabola going through the origin. Now take the line through the origin $y(x) = px$, where p is the slope. Define $x(p)$ as the point at which

$$F(p, x) = y(x) - f(x) = px - f(x) \tag{2.42}$$

is maximum.

Lemma 1. *$x(p)$ is the point at which the tangent to $f(x)$ is parallel to $y(x) = px$.*

Proof. By construction, $x(p)$ is the point that maximizes $F(p, x)$. Therefore it is the point at which $\frac{\partial F}{\partial x} = 0$:

$$\frac{\partial F}{\partial x} = y'(x) - f'(x) = 0$$
$$p - f'(x) = 0 \quad \Rightarrow \quad f'(x) = p.$$

□

If $f(x)$ is convex, $x(p)$ is unique if it exists [2]. The function $F(p, x) = px - f(x)$ is the Legendre transform of $f(x)$, and it happens to equal the negative of the y-intercept of the tangent to $f(x)$ at $x(p)$. However, it is better to think of it as a function of p only, as follows:

1. Pick a convex $f(x)$, as above

2. Define $y = px + b$, as the equation of the tangent to f at x, where b is the y-intercept
3. As stated, $F(p) = px - f(x) = px - y(x) = -b$
4. As we just proved, $p = f'(x)$, which implies that $\quad x = (f')^{-1}(p)$
5. Then, $F(p) = px - f(x) = p\,\left[(f')^{-1}(p)\right] - f\left[(f')^{-1}(p)\right]$.

Let us now apply this recipe to the Lagrangian of the SHO, with the proviso that we are assuming a time-independent Lagrangian and that we are only transforming with respect to the $\dot{q}$ coordinate, q is just carried through unchanged:[12]

1. $L(\dot{q}, q) = T - U = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}kq^2$
2. $y(\dot{q}) = p\dot{q} + b \quad$ is the equation of the tangent to $L(\dot{q}, q)$ at $\dot{q}$, where b is the y-intercept.
3. Define $H(p, q) = -b = p\dot{q} - y(\dot{q}) = p\dot{q} - L(\dot{q}, q)$
4. $p = L'(\dot{q}) = m\dot{q} \qquad \Rightarrow \qquad \dot{q} = (L')^{-1}(p) = \frac{p}{m}$
5. Then,

$$\begin{aligned} H(p, q) &= p\dot{q} - L(\dot{q}, q) = p\big[(L')^{-1}(p)\big] - L\big[(L')^{-1}(p), q\big] \\ &= p\Big[\frac{p}{m}\Big] - L\Big[\frac{p}{m}, q\Big] = \frac{p^2}{m} - \frac{1}{2}m\left(\frac{p}{m}\right)^2 + \frac{1}{2}kq^2 = \frac{1}{2}\frac{p^2}{m} + \frac{1}{2}kq^2, \end{aligned} \tag{2.43}$$

showing that for frictionless systems the Hamiltonian is the Legendre transform of the Lagrangian and the (conserved) total mechanical energy. In the Hamiltonian formulation p and q are called ‘conjugate variables’, or ‘conjugate coordinates’.

2.2.4.3 Hamitonian Formulation

Whereas the solution of the Euler-Lagrange equations (2.41) yields $q(t)$, i.e. trajectories in the $\mathbb{R}^n$ configuration or state space of the system, in the Hamiltonian formulation the state of the system is a point in phase space and it is defined by the tuple $(p, q) \in \mathbb{R}^{2n}$. Therefore, we need $2n$ governing equations. These are easily derived as follows. We calculate the total differential of the Hamiltonian from the expression for the Legendre transform:[13]

$$H = p_i\dot{q}_i - L \tag{2.44}$$

$$\begin{aligned} dH &= \dot{q}_i dp_i + p_i d\dot{q}_i - \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i - \frac{\partial L}{\partial q_i} dq_i - \frac{\partial L}{\partial t} dt \\ &= \dot{q}_i dp_i + p_i d\dot{q}_i - p_i d\dot{q}_i - \dot{p}_i dq_i - \frac{\partial L}{\partial t} dt \\ &= \dot{q}_i dp_i - \dot{p}_i dq_i - \frac{\partial L}{\partial t} dt, \end{aligned} \tag{2.45}$$

where we have used Eq. (2.41) and repeated indices in the same term imply summation from 1 to n (Einstein summation convention). But the total differential of $H(p, q)$ is also given by

$$dH = \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial t} dt. \tag{2.46}$$

Equating terms we get Hamilton’s equations of motion

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i} \qquad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}. \tag{2.47}$$

[12] A proper, coordinate-free, and geometric treatment of contact transformations can be found in Burke [8]. In this brief summary we can only afford to rely on the less satisfactory but easier Goldstein [21].

[13] In this simplified treatment we are not distinguishing between covariant and contravariant vectors by using subscripts and superscripts for the indices as is usually done.

2.2.4.4 Canonical Transformations and Hamilton-Jacobi Equation

We follow Goldstein [21] in this section. From Eq. (2.41) it is clear that if the Lagrangian of a system is not a function of a specific q_i then $\dot{p}_i = 0$ and, therefore, the corresponding momentum p_i will be constant for that system. Generalized coordinates that are absent from the Lagrangian are called 'cyclic', probably because the first ones were found in orbital dynamics where the force field is radial or central, implying that angular momentum is conserved. In central force fields the Lagrangian does not depend on the satellite's angle coordinate θ, the archetypical 'cyclic' variable.

Now consider a problem in which all variables are cyclic. Under these conditions, all the conjugate momenta are constant:

$$p_i = \alpha_i, \tag{2.48}$$

where since we are following Goldstein's notation now α is not an eigenvalue as it was earlier in the chapter but merely a constant of the motion. In such cases, the Legendre transformation (2.44) shows that the Hamiltonian is not a function of the cyclic variables either, but only of the constant conjugate momenta. Therefore $H = H(\alpha_1, \cdots, \alpha_n)$ is constant too. From (2.47) we have that

$$\dot{q}_i = \frac{\partial H}{\partial \alpha_i} = \omega_i, \tag{2.49}$$

are constant too, leading to the trivial solutions

$$q_i(t) = \omega_i t + \beta_i, \tag{2.50}$$

where the β_i are the remaining n constants of integration.

It is clear that a central force problem expressed in Cartesian coordinates does not have any cyclic coordinates, but if it is expressed in polar coordinates θ is cyclic. Further, it is not surprising that central force problems expressed in polar coordinates are easier to work with and solve than when the same problem is expressed in Cartesian or other systems of coordinates. In the context of Hamiltonian dynamics, the process of expressing a given problem into a different set of coordinates that may make it easier to solve is formalized through the method of canonical transformations [21, 2]:

$$Q_i = Q_i(p, q, t) \qquad\qquad P_i = P_i(p, q, t), \tag{2.51}$$

such that

$$\dot{Q}_i = \frac{\partial K}{\partial P_i} \qquad\qquad \dot{P}_i = -\frac{\partial K}{\partial Q_i}, \tag{2.52}$$

where $K(P, Q)$ is the transformed Hamiltonian. How can we be sure that also the new coordinates will be canonical? They need to satisfy Hamilton's principle (2.40), which can be expressed for both old and new variables in terms of the Hamiltonian as

$$\delta \int_{t_1}^{t_2} \big[p_i \dot{q}_i - H(p, q, t)\big]\, dt = 0 \qquad\qquad \delta \int_{t_1}^{t_2} \big[P_i \dot{Q}_i - K(P, Q, t)\big]\, dt = 0. \tag{2.53}$$

However, the integrands of these two integrals do not have to be equal for their variations to vanish. This provides an opening for an algorithmic approach at constructing canonical transformations, as follows. First, we notice that the most general relationship between them is

$$\lambda\big[p_i \dot{q}_i - H(p, q, t)\big] = P_i \dot{Q}_i - K(P, Q, t) + \frac{dF}{dt}, \tag{2.54}$$

where λ is a real constant factor and F is a function of the old and new phase space variables; thus, $F(t)$ is a shorthand for, in general, $F\big(p_i(t), q_i(t), P_i(t), Q_i(t)\big)$. The scale factor changes the LHS uniformly but does not change how the functional depends on the variation function. Thus, it is normally set equal to 1. Similarly, since the additional function F depends on the variables that are being varied and since the variation vanishes at the end points, the integral

$$\int_{t_1}^{t_2} \frac{dF}{dt}\, dt = F(t_2) - F(t_1), \tag{2.55}$$

is constant under variation and does not change the extrema. Second, we restrict F to depend on the same number of old and new variables, but picking only either the positions or the momenta for each. This leads to 4 possible combinations for the functional form of F, which is then called the generating function since with this functional form it acts as a bridge between the old and new variables. We just need to demonstrate one of them to arrive at the intermediate result we need.

Let the generating function depend on the old and new position variables: $F = F_1(q, Q, t)$. Then Eq. (2.54), with $\lambda = 1$, becomes

$$\begin{aligned} p_i \dot{q}_i - H &= P_i \dot{Q}_i - K + \frac{dF_1}{dt} \\ &= P_i \dot{Q}_i - K + \frac{\partial F_1}{\partial q_i}\dot{q}_i + \frac{\partial F_1}{\partial Q_i}\dot{Q}_i + \frac{\partial F_1}{\partial t}. \end{aligned}$$

Rearranging,

$$\left(p_i - \frac{\partial F_1}{\partial q_i}\right)\dot{q}_i - \left(P_i + \frac{\partial F_1}{\partial Q_i}\right)\dot{Q}_i - H + K - \frac{\partial F_1}{\partial t} = 0. \tag{2.56}$$

Since the $\dot{q}_i$ and $\dot{Q}_i$ can vary independently, for this equation to vanish their coefficients must equal zero. In addition, the remaining terms must also add up to zero. Therefore,

$$p_i = \frac{\partial F_1}{\partial q_i}(q, Q, t) \tag{2.57}$$

$$P_i = -\frac{\partial F_1}{\partial Q_i}(q, Q, t) \tag{2.58}$$

$$K(P, Q, t) = H\big(p(P, Q, t), q(P, Q, t), t\big) + \frac{\partial F_1}{\partial t}\big(q(P, Q, t), Q, t\big). \tag{2.59}$$

Eqs. (2.57) are n relations expressing the p_i as functions of (q, Q, t). Assuming they can be inverted, they can be solved for $Q_i(p, q, t)$, which are the first half of Eqs. (2.51). These functions can then be substituted into Eqs. (2.58) to obtain $P_i(p, q, t)$, the second half of Eqs. (2.51). Finally, inverting Eqs. (2.51), we obtain $p(P, Q, t)$ and $q(P, Q, t)$, which are substituted into Eqs. (2.59) to obtain $K(P, Q, t)$ as desired. The reader is referred to [21] for examples and further discussion of the four kinds of transformations. We have introduced them this far to arrive at the next step, the derivation of the Hamilton-Jacobi equation.

A radical use of this theory is to seek a transformation to *constant* position and momentum variables. For example, such constant variables could be the initial conditions (p_0, q_0). In such a case, the reverse transformation would be comprised of functions

$$q = q(p_0, q_0, t) \qquad\qquad p = p(p_0, q_0, t),$$

which are actually the solutions being sought (vector character assumed). This outcome can be achieved by setting the new Hamiltonian $K = 0$ identically since, then,

$$\dot{Q}_i = \frac{\partial K}{\partial P_i} = 0 \qquad\qquad \dot{P}_i = \frac{\partial K}{\partial Q_i} = 0.$$

As we saw above in Eqs. (2.59),

$$K = H + \frac{\partial F_1}{\partial t}, \tag{2.60}$$

so that we want, dropping the subscript on F,

$$H(p,q,t) + \frac{\partial F}{\partial t} = 0. \tag{2.61}$$

This works for other choices of F as well. So we choose a generating function that depends on the old position coordinates q_i and the new constant momenta P_i, and call it S instead of F. The analogue of Eqs. (2.57) are

$$p_i = \frac{\partial S}{\partial q_i}(q,P,t), \tag{2.62}$$

such that Eq. (2.61) becomes

$$\boxed{H\left(\frac{\partial S}{\partial q_1},\cdots,\frac{\partial S}{\partial q_n},q_1,\cdots,q_n,t\right) + \frac{\partial S}{\partial t} = 0.} \tag{2.63}$$

This is the Hamilton-Jacobi equation (HJE), and S is called Hamilton's principal function. It is not difficult to show (see e.g. [1]: 96) that the Hamilton equations (2.47) plus the definition of the action (2.39) expressed in differential form constitute the characteristic equations for this PDE, which is why we use the same symbol S for the action and for the principal function. They are indeed the same function. We now need to derive the Hamilton-Jacobi-Bellman equation (HJBE), which is closely related to the HJE and for systems of stochastic differential equations (SDEs) provides the governing PDE for the quasi-potential.

2.2.4.5 The Principle of Optimality

Richard Bellman generalized the calculus of variations to the numerical analysis of optimization problems, and in particular optimal control problems. This generalization was motivated in part by the fact that in many situations optimal control problems are expressed mathematically as boundary-value problems, which are much more difficult to solve numerically than initial value problems, especially if they are non-linear [5]. In addition, Bellman showed how this theory is also relevant to the solution of SDEs [4], such that his formulation has remained to this day the standard starting point in this area of statistical physics and stochastic modelling (e.g. [18, 51, 9]).

As often happens when one field (in this case, Lagrangian dynamics and calculus of variations) branches off into different theoretical and applied fields (in this case, optimal control theory, discrete optimization, stochastic modelling in biology and physics), or is even applied in different disciplines (in this case, economics and game theory), the web of bibliographical references gets very complicated and the use of terms of art bifurcates into different sub-dialects. A good example of this is the fact that in the derived and applied literature in control theory the HJE is often referred to as the HJBE, whereas it isn't, it is the same HJE. What's different, however, is the principle from which it is derived, the principle of optimality, which is indeed more general than Hamilton's principle.

Before starting with the derivations, therefore, it is helpful to clarify the relationship between the application of the calculus of variations to Lagrangian dynamics and problems in optimal control: the former are a subset of the latter. This can be easily seen by drawing on Gelfand and Fomin [19], who define the following concepts. Let $x \in \mathbb{R}^n$ represent the state of a system in configuration space, whose time evolution is governed by a set of ODEs:

$$\dot{x}^i = f^i(x^1,\cdots,x^n,u^1,\cdots,u^k), \qquad i=1,\cdots,n \qquad \text{and} \qquad u \in \Omega \subset \mathbb{R}^k. \tag{2.64}$$

Here u is a k-dimensional vector of parameters whose admissible values fall within the set Ω. By standard existence and uniqueness theorems of differential equations, defining the control function $u(t)$ over the interval $t_0 \le t \le t_1$ ensures that $\dot{x}^i = f^i(x^1,\cdots,x^n,u^1(t),\cdots,u^k(t))$ has a unique solution or trajectory in configuration space over this interval. Now define the control process

$$U = \{u(t), t_0, t_1, x_0\}, \tag{2.65}$$

a suitably continuous additional function $f^0(x^1, \cdots, x^n, u^1, \cdots, u^k)$, and the functional

$$J(U) = \int_{t_0}^{t_1} f^0(x, u)\, dt, \qquad J \in \mathbb{R}. \tag{2.66}$$

U is optimal if $J(U)$ is minimum relative to any other U^* that maps a given $x_0(t_0)$ to $x_1(t_1)$. The control function $u(t)$ that gives an optimal control process U is called an *optimal policy.*

With these definitions, to get Lagrangian dynamics we just need to let

$$J(U) = \int_{t_0}^{t_1} f^0(x^1, \cdots, x^n, u^1, \cdots, u^n)\, dt, \qquad \text{with} \qquad \dot{x}^i = u^i, \qquad i = (1, \cdots, n), \tag{2.67}$$

where now $f^0 = L$ (the Lagrangian), $J(U) = S$ (the action), $u = \dot{x}$ is the velocity vector, and both x and u range over n dimensions. Clearly this is more restrictive than the general optimal control problem above.

The fundamental idea of dynamic programming is to turn the calculus of variation problem around and solve something that could be regarded as its inverse. Bellman [3] started with a generalization of Hamilton's principle (2.39):

$$\text{Minimize} \int_0^t F(x, z)\, du \tag{2.68}$$

subject to

$$\frac{dx}{du} = G(x, z), \qquad x(0) = c, \tag{2.69}$$

where c is the initial value of the minimizing function and t is end-point of the interval over which the functional is minimized. When $G(x, z) = z$, z becomes the velocity, F becomes the Lagrangian, and this functional reverts to the familiar principle (2.39). Rather than fixing c and t and seeking a function $x(u)$ that minimizes the functional, we seek $z(0)$ as a function of c and t.[14] Thus, we seek

$$f(c, t) = \min_z \int_0^t F(x, z)\, du, \tag{2.70}$$

where $f(c, t)$ is called the 'value' function. A second way in which Bellman's optimization is "backwards" is that 'in place of determining the optimal *continuation* from one fixed position, we try to find the optimal *first step* from any position' ([3], emphasis added). This is achieved by (1) breaking up the domain into two parts; (2) fixing the second; (3) optimizing the first; and (4) letting its length go to zero. The result is an optimum initial value for a given subsequent development. The formalism ensures that the 'given' subsequent development is also optimal. This process is then applied recursively over many steps, backwards from the end point towards the initial point.

Thus, we introduce the multi-stage optimization:

$$f(c, s + t) = \min_z \int_0^{s+t} F(x, z)\, du = \min_z \left[\int_0^s F(x, z)\, du + \int_s^{s+t} F(x, z)\, du \right]. \tag{2.71}$$

With a slight abuse of notation, whereas the initial condition for the first segment is $x(0) = c$, for the second segment we use $x(s) = c(s)$, which just signifies a different value of x expressed as a parameter whose value depends on the location of the boundary point s between the two intervals. Whatever we do with the first segment, i.e. whichever $z(u)$ we choose, the second segment will need to be optimized subject to the constraint (2.69) and initial condition $x(s) = c(s)$. Since the constraint ODE (2.68)

[14] Notice that, in the simple mechanics case, this is analogous to seeking the initial slope of the numerical solution in the so-called 'shooting method' of numerical analysis of boundary-value problems.

is autonomous and the integrand of (2.68) does not depend on time, the optimization problem is invariant with respect to time translations. Therefore, we can also say that

$$f(c(s), t) = \min_z \int_s^{s+t} F(x, z)\, du, \tag{2.72}$$

such that

$$\boxed{f(c, s+t) = \min_{z[0,s]} \left[\int_0^s F(x, z)\, du + f(c(s), t) \right].} \tag{2.73}$$

The notation $z[0, s]$ indicates that the optimization is over all $z(u)$ in the interval $0 \le u \le s$. This is the functional equation form of the principle of optimality, as derived in [4], which can be stated in words as:

> An optimal policy has the property that, whatever the initial state and initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision. [4]

Although the dependence of Eq. (2.73) on the initial state is not very visible, yet, the recursive nature of the principle is already evident since the second term refers to an already-optimized second interval expressed as a function of *its* initial state, $c(s)$.

2.2.4.6 The Hamilton-Jacobi-Bellman Equation

For the next stage of the derivation it is better to use reference [5] and a slightly different problem formulation. Consider the minimization of the functional

$$J(x) = \int_a^b F(t, x, \dot{x})\, dt, \tag{2.74}$$

with the initial condition $x(a) = c$. This time, the minimum of this functional is expressed as a function of the *initial* t-value a and initial x-value c. Application of the principle of optimality just derived yields the functional equation

$$f(a, c) = \min_{x[a, a+\Delta]} \left[\int_a^{a+\Delta} F(t, x, \dot{x})\, dt + f(a + \Delta, c(x)) \right]. \tag{2.75}$$

Here Δ plays the same role as s in the previous derivation, $x[a, a + \Delta]$ signifies that the minimizing function $x(t)$ should be sought in the interval shown, the second term concerns the second interval $[a + \Delta, b]$, and $c(x) = x(a + \Delta)$. We assume that $f(a, c)$ has continuous first and second partial derivatives. Note also that choosing $x(t)$ in the first interval $[a, a + \Delta]$ subject to the constraint that $x(a) = c$ is equivalent to choosing $\dot{x}(t)$ in the same interval. If we let $\Delta \to 0$ this, in turn, is equivalent to choosing $\dot{x}(a)$. Thus, expanding the right-hand side (RHS) of the above equation in a Taylor series about a,

$$\begin{aligned}
f(a, c) &= \min_{\dot{x}(a)} \left\{ \int_a^a F(t, x, \dot{x})\, dt + \frac{d}{dt} \left[\int_a^{a+\Delta} F(t, x, \dot{x})\, dt \right]_a \Delta + \cdots + f(a + \Delta, c + \dot{x}(a)\Delta) \right\} \\
&= \min_{\dot{x}(a)} \left\{ F(a, c, \dot{x}(a))\Delta + f(a, c) + \frac{\partial f}{\partial a}\Delta + \left[\frac{\partial f}{\partial c} \frac{dx}{dt} \right]_a \Delta \right\} \\
&= \min_{\dot{x}(a)} \left\{ F(a, c, \dot{x}(a))\Delta + f(a, c) + \frac{\partial f}{\partial a}\Delta + \frac{\partial f}{\partial c}\dot{x}(a)\Delta \right\}.
\end{aligned}$$

Simplifying,

$$0 = \min_{\dot{x}(a)} \left\{ F(a, c, \dot{x}(a)) + \frac{\partial f}{\partial a} + \frac{\partial f}{\partial c}\dot{x}(a) \right\}.$$

Reverting to general variables ($a = t$, $c = x$, $\dot{x}(a) = \dot{x}$),

$$0 = \min_{\dot{x}} \left\{ F(t, x, \dot{x}) + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\dot{x} \right\}.$$

The minimization of this quantity is equivalent to enforcing two separate equations. The first is the vanishing of the partial derivative of this quantity w.r.t. $\dot{x}$, since we are looking for an extremum and we are varying $\dot{x}$, and the second is the equation itself since for any choice of $\dot{x}(t)$ the equation must still equal zero:

$$\frac{\partial F}{\partial \dot{x}} + \frac{\partial f}{\partial x} = 0 \tag{2.76}$$

$$F(t, x, \dot{x}) + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\dot{x} = 0. \tag{2.77}$$

If we now make the identification $F = L$ and $f = S$,

$$\frac{\partial S}{\partial x} = -\frac{\partial L}{\partial \dot{x}} = -p \tag{2.78}$$

$$L(t, x, \dot{x}) + \frac{\partial S}{\partial t} - p\dot{x} = 0. \tag{2.79}$$

Using the Legendre transformation (2.44), we get

$$p\dot{x} - H + \frac{\partial S}{\partial t} - p\dot{x} = 0$$

$$H - \frac{\partial S}{\partial t} = 0. \tag{2.80}$$

This is close to but not quite the same as the HJE (2.63). What happened? The derivation of the HJE shown in [5] sheds some light. As we will see below, however, what we have done here is also relevant, in a different way.

To derive the HJE, Bellman and Dreyfus [5] apply the principle of optimality at *both* ends of the interval. The crucial insight is that, as we have derived earlier with the canonical transformations, the HJE is expressed in terms of the *source* variables of the transformation, where the *target* variables are instead the (constant) initial conditions. This is visible in Eq. (2.60). In the present context this means that we need to derive the differential equation for the value function (f, or the action S) by applying the principle of optimality at the other (right) end of the interval, not at the beginning of the interval where the initial conditions are. Thus, we proceed by defining the action as

$$S(q, t; Q, t_0) = \min \int_{t_0}^{t} L(q, \dot{q}, t_1)\, dt_1, \tag{2.81}$$

where q is the state vector and Q is its initial value at time t_0. Application of the principle of optimality at both ends yields two conditions:

$$S(q, t; Q, t_0) = \min_{\dot{Q}(t_0)} \left[L(Q, \dot{Q}, t_0)\Delta + S(q, t, Q + \dot{Q}\Delta, t_0 + \Delta) \right] \tag{2.82}$$

$$S(q, t; Q, t_0) = \min_{\dot{q}(t)} \left[L(q, \dot{q}, t)\Delta + S(q - \dot{q}\Delta, t - \Delta, Q, t_0) \right]. \tag{2.83}$$

Expanding in a Taylor series at both ends of the interval and simplifying,

$$0 = \min_{\dot{Q}} \left[L + \dot{Q}\frac{\partial S}{\partial Q} + \frac{\partial S}{\partial t_0} \right] \tag{2.84}$$

$$0 = \min_{\dot{q}} \left[L - \dot{q}\frac{\partial S}{\partial q} - \frac{\partial S}{\partial t} \right]. \tag{2.85}$$

As above, this leads to 2 conditions at each end:

$$0 = L + \dot{Q}\frac{\partial S}{\partial Q} + \frac{\partial S}{\partial t_0} \tag{2.86}$$

$$0 = L - \dot{q}\frac{\partial S}{\partial q} - \frac{\partial S}{\partial t} \tag{2.87}$$

and

$$\frac{\partial L}{\partial \dot{Q}} = -\frac{\partial S}{\partial Q} = P \tag{2.88}$$

$$\frac{\partial L}{\partial \dot{q}} = \frac{\partial S}{\partial q} = p. \tag{2.89}$$

Substituting (2.88) and (2.89) in (2.86) and (2.87), respectively, and using (2.44),

$$P\dot{Q} - K + P\dot{Q} + \frac{\partial S}{\partial t_0} = 0 \qquad \rightarrow \qquad \frac{\partial S}{\partial t_0} = 0 \tag{2.90}$$

$$p\dot{q} - H - p\dot{q} - \frac{\partial S}{\partial t} = 0 \qquad \rightarrow \qquad H + \frac{\partial S}{\partial t} = 0, \tag{2.91}$$

where, since K and $\dot{Q}$ are zero by construction, the first equation just yields the initial condition for S, and the second is the desired HJE.

We went through all these details and derivations because there is a strange inconsistency between the HJE cited in the SDE literature [18, 10, 23, 9, 51] and the HJE equation derived here. Namely, the SDE literature uses a form of the HJE that is consistent with (2.77) or (2.86), which seems problematic. Let us show how, and then propose a possible way to explain or justify this choice.

2.3 The Stochastic Perspective

2.3.1 A Different Form of HJE

The form of the HJE used in [18], which is one of the standard references for stochastic modelling research (e.g. [10, 23, 9, 51]), is

$$\frac{\partial S}{\partial t} + \frac{1}{2}|\boldsymbol{\nabla} S|^2 + \boldsymbol{\nabla} S \cdot \boldsymbol{b}(\boldsymbol{x}) = 0, \tag{2.92}$$

where in line with physics convention we are using boldface to emphasize vector character, $\boldsymbol{b}(\boldsymbol{x})$ is the 'drift force' vector field representing the RHS of a system of 1st-order ODEs, and $\boldsymbol{\nabla}$ is the symbol for the gradient operator. The space in which this PDE for the scalar function $S(\boldsymbol{x})$ applies is $\mathbb{R}^n$, where n is the number of ODEs in the system or the number of dependent variables (for example, chemical species concentrations). However, in [18] and related references the quasi-potential U is used in place of S in the above equation. The reason, to be explained in more detail below, stems from the fact that Freidlin and Wentzell define a particular kind of action that applies to stochastic systems and that is proportional to a probabilistically defined 'quasi-potential'. Here we want to focus on linking this equation to Hamilton-Jacobi theory as a prerequisite for the derivations and discussions to follow.

If we envisage the HJE derived in the previous section to apply in $\mathbb{R}^n$ rather than in one dimension, then using (2.89) and the fact that the drift force vector equals the vector of first derivatives of the dependent variables (merely by how a system of 1st-order ODEs is formulated), we get

$$\frac{\partial S}{\partial t} + \frac{|\boldsymbol{p}|^2}{2} + \boldsymbol{p} \cdot \dot{\boldsymbol{x}} = 0, \tag{2.93}$$

But $\frac{|\boldsymbol{p}|^2}{2}$ is the kinetic energy/unit mass. Since the potential energy term is neglected in stochastic processes such as Brownian motion, this term could be either the Hamiltonian or the Lagrangian. If we assume it's the latter, we can rewrite the equation as

$$L + \boldsymbol{p} \cdot \dot{\boldsymbol{x}} + \frac{\partial S}{\partial t} = 0, \tag{2.94}$$

which is the same form as Eq. (2.86)'s.

As we saw above, if we apply a Legendre transformation to the Lagrangian in the above equation, to express the problem in terms of the conjugate variables, we get the "wrong" HJE. Alternatively, if we interpret the gradient-squared term as the Hamiltonian, directly, then the resulting equation is inconsistent with Hamilton-Jacobi theory. The best explanation or justification we can offer is that the Freidlin and Wentzell large-deviation theory of stochastic processes is concerned with meta-stable states, where systems are envisaged to spend most of their time at or near an equilibrium point, and only rarely venture far enough away possibly to transition to a new meta-stable state. As a consequence, it appears to be a theory that is mostly based on the *starting point* of a time evolution. This would justify using the Bellman equation (principle of optimality) near the *origin* rather than at some arbitrary point, where the origin is identified with a given equilibrium or meta-stable point in phase space. This is then what we are going to assume going forward.

As a point of critique of interdisciplinary communications, it is remarkable that so little foundational information is provided in Freidlin and Wentzell's otherwise excellent book – and that most practitioners in this field do not question this form of the HJE. No matter. We now feel we have a sufficiently good intuitive and mathematical understanding of the HJE to press forward. Our next tasks are (1) to extend our understanding of differential equations to stochastic differential equations and (2) to provide a brief but sufficiently detailed introduction to probability theory to enable us to understand the quasi-potential formalism in the context of large deviation theory. These two points together will also enable us to understand how and why Hamiltonian dynamics can possibly be relevant to dissipative cell metabolic systems.

2.3.2 Stochastic Differential Equations

The prototypical problem of interest to us is physical Brownian motion as described by Langevin's equation [46]. Langevin's equation is an SDE where the stochasticity is introduced to model motion on a fast time-scale, whereas the slow time-scale motion is driven by the familiar force terms in Newton's law:

$$\mu \ddot{q} = -\dot{q} + b(q) + \sqrt{\epsilon}\sigma(q)\dot{w}, \tag{2.95}$$

where μ is the mass of the particle, q is a generalized coordinate in $\mathbb{R}^n$ (where $n = 3$ for actual Brownian motion), $\dot{q}$ is the velocity-dependent frictional force,[15] $b(q)$ is a force vector field, ϵ is a small number (and the square-root is just for later convenience), σ is the diffusion $n \times n$ matrix, and $\dot{w}$ is Gaussian white noise. We are assuming vector character for the dependent variable, but since in this case we feel that there is less opportunity of confusing the symbols with what came before we are not using boldface.

As explained by Chen [10], the Smoluchowski-Kramers approximation of Langevin's equation consists in the statement that as the mass μ of the particle approaches zero the solution of Eq. (2.95) approaches the solution of the same equation without the highest derivative term:

$$\dot{q} = b(q) + \sqrt{\epsilon}\sigma(q)\dot{w}. \tag{2.96}$$

[15] The damping or friction coefficient is set equal to 1 for simplicity, so the units of $\dot{q}$ can actually be Newtons, depending on context.

This turns the original 2nd-order problem into a 1st-order diffusion problem and is the reason why the RHS of systems of 1st-order ODEs modelling cell metabolic and regulatory systems is called the 'drift force'. It's because by analogy with Brownian motion it can truly be claimed to be a force vector field.

The literature now splits into problems for which the force vector field $b(q)$ is the gradient of a potential and problems for which it is not. We will focus on the latter, which result from dissipative systems. Before we cover the basics of large deviation theory, however, it is helpful to review more fundamental material. Accordingly, in the next section we introduce a few basic concepts from probability theory with which we can derive the Master equation, which in turn is the reference point for the Fokker-Planck equation and the Langevin equation.

2.3.3 The Master Equation

The material in this section is taken mainly from [46].

2.3.3.1 Basic Definitions

A *stochastic variable* X is a variable that can take on values from a given range with a given probability distribution. A stochastic *process* is a stochastic variable that is defined as a function of X and t:

$$Y_X(t) \colon \mathbb{R}^2 \to \mathbb{R}, \qquad\qquad Y_X(t) = f(X,t), \tag{2.97}$$

where we follow van Kampen's notation. A *sample function* or realization is obtained by inserting a particular value $x \in X$

$$Y_x(t) = f(x,t), \tag{2.98}$$

such that x is necessarily fixed. Each x defines a different physical process that started with that value. Therefore, the whole set is an ensemble, as shown in Figure 2.7. Note that intuitively we might expect the values of $Y_x(t)$ for times $t > 0$ to come from the stochastic variable X. However, if this were the case then the sample function could not be a simple "slice" parallel to the t axis, as shown in Figure 2.7, but would have to vary in the X direction as well. Therefore, if $Y_x(t)$ is to be an 'ordinary function of t', as van Kempen says ([46]: 52), x should be seen simply as a way to distinguish the different members of the ensemble, thereby playing the role of an index. Because a stochastic process takes place in time, and because at each point in time the value of a sample function can change, the concepts of 'state' and 'event' are similarly relevant for indicating a given value of $Y_x(t)$, and in the following we may use them interchangeably.

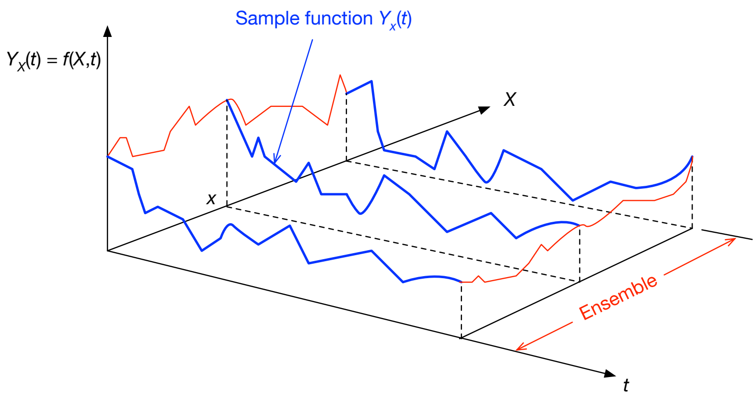

Fig. 2.7: **Ensemble of sample functions of a stochastic process**

We define a *probability density* $P_X(x)$ over the values of X, such that the ensemble average or *expectation value* of the stochastic process is a function of time given by

$$\langle Y(t)\rangle = \int Y_x(t) P_X(x) dx. \tag{2.99}$$

This is potentially confusing, since we just said that x is just playing the role of an index. Therefore, is it correct to define a probability distribution over the values of an index? It would appear so, since the effect of such a distribution is simply to select different sample functions depending on the probability of the value of x with which they are associated to occur. The implication is that $P_X(x)$ is not a function of time, as indeed its functional signature suggests. The *nth moment* is defined as

$$\langle Y(t_1)Y(t_2)\cdots Y(t_n)\rangle = \int Y_x(t_1)Y_x(t_2)\cdots Y_x(t_n) P_X(x) dx, \tag{2.100}$$

where $t_1, t_2, \cdots t_n$ are not necessarily all different (Figure 2.8). The *autocorrelation function* is defined

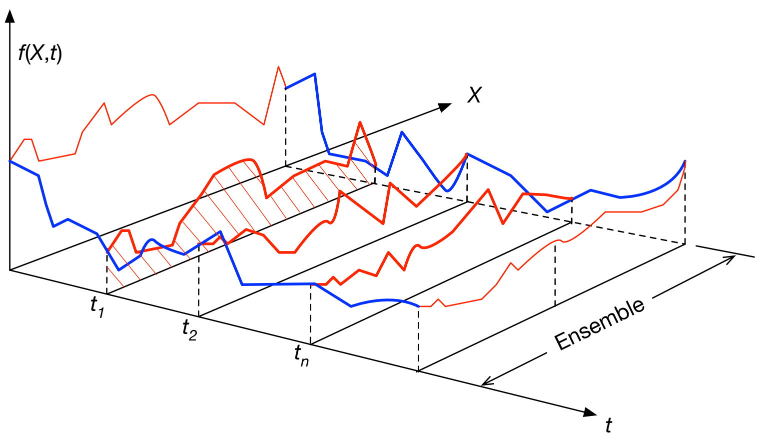

Fig. 2.8: **Calculation of nth moment**

as the expectation value of the second central moment:

$$\kappa(t_1, t_2) = \langle\langle\ Y(t_1)Y(t_2)\ \rangle\rangle = \Big\langle\ \big[\ Y(t_1) - \langle Y(t_1)\rangle\ \big]\ \big[\ Y(t_2) - \langle Y(t_2)\rangle\ \big]\ \Big\rangle, \tag{2.101}$$

where the double angle brackets do not signify taking the expectation value twice but indicate a different type of bracket whose meaning is defined by this equation. If $t_1 = t_2$ we get the familiar expression for the *variance*:

$$\begin{aligned}
\langle\langle\ Y(t)^2\ \rangle\rangle &= \Big\langle\ \big(\ Y(t) - \langle Y(t)\rangle\ \big)^2\ \Big\rangle && (2.102)\\
&= \Big\langle\ Y(t)^2 - 2Y(t)\langle Y(t)\rangle + \langle Y(t)\rangle^2\ \Big\rangle\\
&= \langle Y(t)^2\rangle - 2\big\langle Y(t)\ \langle Y(t)\rangle\big\rangle + \big\langle\langle Y(t)\rangle^2\big\rangle\\
&= \langle Y(t)^2\rangle - 2\langle Y(t)\rangle\ \langle Y(t)\rangle + \langle Y(t)\rangle^2\\
&= \langle Y(t)^2\rangle - \langle Y(t)\rangle^2. && (2.103)
\end{aligned}$$

Similarly, a simple calculation shows that Eq. (2.101), the autocorrelation in terms of the second *central* moment, can be expressed in terms of the second moment and the expectation values:

$$\kappa(t_1, t_2) = \langle\langle\ Y(t_1)Y(t_2)\ \rangle\rangle = \langle Y(t_1)Y(t_2)\rangle - \langle Y(t_1)\rangle\langle Y(t_2)\rangle. \tag{2.104}$$

A stochastic process is *stationary* if the moments are not affected by a shift in time:

$$\big\langle Y(t_1+\tau)Y(t_2+\tau)\cdots Y(t_n+\tau)\big\rangle = \big\langle Y(t_1)Y(t_2)\cdots Y(t_n)\big\rangle. \tag{2.105}$$

If $Y(t)$ is a vector, then the $\kappa(t_1, t_2)$ is a matrix whose entries are:

$$\kappa_{ij}(t_1, t_2) = \langle\langle\ Y_i(t_1)Y_j(t_2)\ \rangle\rangle \tag{2.106}$$

Thus, the diagonal terms are autocorrelations, while the off-diagonals are called *cross-correlations.*

2.3.3.2 Multivariate Distributions

Let X be a random variable with r components $X = (X_1, X_2, \cdots, X_r)$, so $X \in \mathbb{R}^r$. Its probability density is a function $P_r(x_1, x_2, \cdots, x_r)\colon \mathbb{R}^r \to U$, with $U = [0,1] \subset \mathbb{R}$. P_r is called the *joint probability distribution* (JPD) of the r (component) variables. As a notational point, the subscript of the probability function P indicates the number of arguments upon which the probability depends.

Take a subset $(X_1, X_2, \cdots, X_s) \in \mathbb{R}^s$, with $s < r$. The probability that they have values $(x_1, x_2, \cdots, x_s)$ is called the *marginal distribution*:

$$\underbrace{P_s(x_1, x_2, \cdots, x_s)}_{\substack{\text{function of } (x_1, x_2, \cdots, x_s) \\ \text{so distribution over first } s}} = \underbrace{\int P_r(x_1, x_2, \cdots, x_r)dx_{s+1}dx_{s+2}\cdots dx_r,}_{\text{dependence on } s\cdots r \text{ integrated away}} \tag{2.107}$$

where integration over the whole domain of each independent variable being integrated is implied, and all probabilities are always assumed to be normalized over their domains of definition. Therefore, the value of P_s at a particular point $(x_1, \cdots, x_s)$ is larger than $P_r(x_1, \cdots, x_s, x_{s+1}, \cdots, x_r)$, for the same tuple $(x_1, \cdots, x_s)$.

If, instead, we pick a specific set of values for $(x_{s+1}, x_{s+2}, \cdots, x_r)$, the JPD of the rest is called the *conditional probability*: $P_{s|r-s}(x_1, \cdots, x_s|x_{s+1}, \cdots, x_r)$. Note that also in this case the value of $P_{s|r-s}(x_1, \cdots, x_s|x_{s+1}, \cdots, x_r)$ for any given tuple $(x_1, \cdots, x_s)$ is larger than $P_r(x_1, \cdots, x_r)$, for the same tuple. With these definitions, it is self-evident that

$$P_r(x_1, \cdots, x_r) = P_{r-s}(x_{s+1}, \cdots, x_r)P_{s|r-s}(x_1, \cdots, x_s|x_{s+1}, \cdots, x_r). \tag{2.108}$$

This is Bayes's rule, usually expressed as

$$P_{s|r-s}(x_1, \cdots, x_s|x_{s+1}, \cdots, x_r) = \frac{P_r(x_1, \cdots, x_r)}{P_{r-s}(x_{s+1}, \cdots, x_r)}. \tag{2.109}$$

2.3.3.3 Markov Processes and the Chapman-Kolmogorov Equation

The defining characteristic of Markov processes is that the transition probability between two states depends only on the starting state of the transition and not on the history of the process that took place before that point. This is expressed mathematically as

$$P_{1|n-1}(y_n, t_n|y_1, t_1; y_2, t_2; \cdots; y_{n-1}, t_{n-1}) = P_{1|1}(y_n, t_n|y_{n-1}, t_{n-1}). \tag{2.110}$$

This is saying that the probability of the next state of a process given fixed values for all preceding states is actually only dependent on the state immediately preceding the next state. $P_{1|1}$ is called the *transition probability.* The Chapman-Kolmogorov equation (CKE) is derived by making use of Bayes's rule and of the Markov property:

$$\begin{aligned} P_3(y_1, t_1; y_2, t_2; y_3, t_3) &= \overbrace{P_2(y_1, t_1; y_2, t_2)P_{1|2}(y_3, t_3|y_1, t_1; y_2, t_2)}^{\text{Bayes}} \\ &= \underbrace{P_1(y_1, t_1)P_{1|1}(y_2, t_2|y_1, t_1)}_{\text{Bayes}}\underbrace{P_{1|1}(y_3, t_3|y_2, t_2).}_{\text{Markov}} \end{aligned} \tag{2.111}$$

Now integrate both sides over all possible values of y_2, such that y_2 drops out of the LHS:

$$P_2(y_1, t_1; y_3, t_3) = P_1(y_1, t_1) \int P_{1|1}(y_2, t_2|y_1, t_1)P_{1|1}(y_3, t_3|y_2, t_2)dy_2. \tag{2.112}$$

Dividing by $P_1(y_1, t_1)$ and applying Bayes's rule we obtain the CKE:[16]

$$P_{1|1}(y_3, t_3|y_1, t_1) = \int P_{1|1}(y_3, t_3|y_2, t_2)P_{1|1}(y_2, t_2|y_1, t_1)dy_2. \tag{2.113}$$

Any initial probability distribution P_1 and recursively applicable transition probability $P_{1|1}$ will define a Markov process if they satisfy the above equation and the self-evident condition

$$P_1(y_2, t_2) = \int P_{1|1}(y_2, t_2|y_1, t_1)P_1(y_1, t_1)dy_1. \tag{2.114}$$

2.3.3.4 Probabilistic Ontological Expansion

Consistently with the definition of stationary processes, above, a Markov process whose moments are affected by a time translation is non-stationary. Another characteristic of stationary Markov processes is that their transition probability depends only on the time difference between states, rather than on the specific times of the two states. There is a particular kind of non-stationary Markov process that is non-stationary only because it starts at a specific time t_0, since translations to times before t_0 are meaningless (see Figure 2.9). Markov processes that are non-stationary due to the fact that they begin at a specified time but whose transition probability after this time only depends on the time difference are called *homogeneous*. The relevance of homogeneous Markov processes comes, for example, from physical systems that are prepared in a non-equilibrium state and then allowed to evolve in time back towards equilibrium. We develop the formalism since it corresponds to the kinds of initial value problems we are interested in investigating.

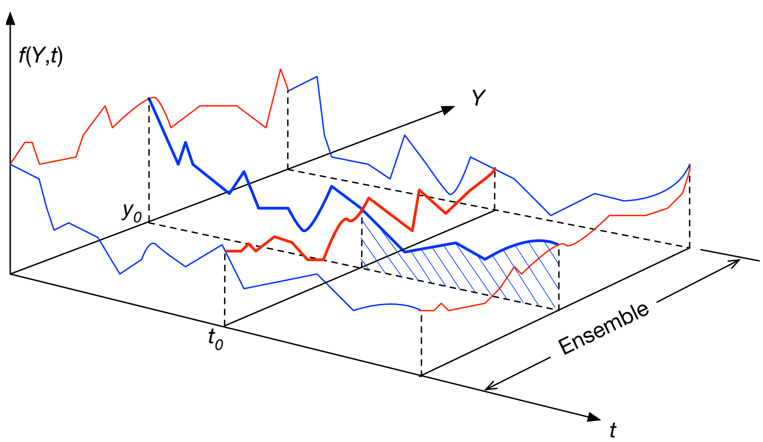

Fig. 2.9: **Visualizing a non-stationary, homogeneous Markov process**

Since homogeneous Markov processes depend only on the time difference between states, the notation to describe them is simpler:

$$P_{1|1}(y_2, t_2|y_2, t_2) = T_\tau(y_2|y_1), \qquad \tau = t_2 - t_1, \tag{2.115}$$

such that the CKE can be written more simply as

$$T_{\tau+\tau'}(y_3|y_1) = \int T_{\tau'}(y_3|y_2)T_\tau(y_2|y_1)dy_2. \tag{2.116}$$

[16] Interestingly, this equation can be seen as the closure condition for the contraction semigroup of a suitably defined family of Markov processes. This is discussed more fully in Chapter 1 of [18], who build on Dynkin's work on Markov processes.

In order to work with these homogeneous processes, van Kampen introduces a seemingly innocuous definition which, however, has important ontological implications. He says that we need to 'extract a sub-ensemble', and that the way we are going to do that is by picking a particular probability distribution $P(y_0)$, where y_0 is allowed to range over all the values of the random variable Y, as before. A simple-minded interpretation of a 'sub-ensemble' is a discrete or continuous subset of the possible values the random variable Y can take on. But this is not what van Kampen means. He means to take the whole range of possible values of Y, but still calls it a subset. The reason is that by defining a probability distribution over Y the ontology of this mathematical quantity is *expanded*: the stochastic variable Y is not only a determinisitc set of possible values, but also an infinite set of possible probability distributions over this set. Having expanded the ontological nature of the original set to include not only the *values* of Y but also *all the possible probability distributions that such values will occur*, the ensemble has become a much larger set. Therefore, it makes sense to call one particular probability distribution a 'subset' of the ensemble.

The reason this point is important is that there are many problems in physics where a deterministic description does not lead to a solvable mathematical problem, but where if the problem is recast in terms of probability a solution can often be obtained. The most obvious example is the position of particles that are small enough for quantum mechanical effects to be important. Heisenberg's uncertainty principle makes it impossible to determine either the position or the momentum exactly, so that a probabilistic description is necessary. It is also very effective and for simple geometries leads to exact solutions that yield a lot of physical insight. Interestingly, an analogous concept appears to apply to macroscopic problems that have too many degrees of freedom to afford an analytical solution, such as happens in the stochastic modelling of chemical reactions. More subtly, there is also a class of dynamical systems that are low-dimensional, such as the metabolic and regulatory pathways we have been studying in BIOMICS, but that are not amenable to analytical solutions by elementary functions. The extension of such ODE models with a stochastic noise component gives valuable additional insight, as in the case of the quasi-potential. With this additional motivation we can carry on with the derivation of the Master equation.

Let a stationary Markov process be given by $P_1(y_1)$ and $T_\tau(y_2|y_1)$. Pick a t_0 and a y_0 and define a new non-stationary but homogeneous Markov process $Y^*(t)$ for $t \geq t_0$:

$$P_1^*(y_1, t_1) = T_{t_1 - t_0}(y_1|y_0) \tag{2.117}$$

$$P_{1|1}^*(y_2, t_2|y_1, t_1) = T_{t_2 - t_1}(y_2|y_1). \tag{2.118}$$

However, it is better to define such a process based on an ensemble. This is where we extract a sub-ensemble by choosing a probability distribution for the initial state:

$$P_1^*(y_1, t_1) = \int T_{t_1 - t_0}(y_1|y_0)p(y_0)dy_0 \tag{2.119}$$

while the transition probability is the same as before. The use of y_0 rather than simply y in the integral is not strictly necessary but it a useful reminder that in this process everything starts at t_0.

Consider a homogeneous Markov process. The Master equation is derived by letting $\tau' \to 0$ in the CKE (2.116). Before we can do that, however, we have to develop an expression for $T_{\tau'}$ as $\tau' \to 0$. For this, we look at radioactive decay as a Markov process.

2.3.3.5 Radioactive Decay

Let n_0 be the number of nuclei of a radioactive material at $t = 0$. Its decay is a combination of mutually independent decay events of individual nuclei. Therefore, the usual argument is to say that the rate of decay is proportional to the number of nuclei present that have not decayed yet, $N(t)$:

$$\frac{dN}{dt} = -\gamma N, \tag{2.120}$$

where γ is a constant, such that

$$N(t) = n_0 e^{-\gamma t}. \tag{2.121}$$

This elementary solution does not highlight the fact that such a decay process satisfies the Markov property. In order to develop an expression for $T_{\tau'}$ as $\tau' \to 0$, we need to recast the radioactive decay process as a Markov process:

$$N(t_2), \text{ conditional on } N(t_1) = n_1, \text{ does not depend on } t < t_1.$$

Let w be the probability that a nucleus survives to time t_1. Then, by a relatively simple argument we have that

$$P(n_1, t_1) = \binom{n_0}{n_1} (1-w)^{n_0 - n_1} w^{n_1}. \tag{2.122}$$

This can be justified intuitively by saying that since the decay events are independent the probability that n_1 have survived is just the product of n_1 individual probabilities, or w^{n_1}. For this outcome to be true it must happen *by the same time* t_1 that the rest of the nuclei *do* decay. This gives the factor $(1-w)^{n_0-n_1}$. The binomial coefficient in front is just due to the fact that there are that many ways to choose n_1 non-decaying nuclei out of the initial n_0. If we define $v = 1 - w$ and treat it as an independent variable, the expectation value of $N(t)$ at $t = t_1$ is given by the average of all possible values of n_1 weighted by the probability of each:

$$\begin{aligned}
\langle N(t_1) \rangle &= \sum_{n_1=0}^{n_0} n_1 \binom{n_0}{n_1} (1-w)^{n_0-n_1} w^{n_1} \\
&= \sum_{n_1=0}^{n_0} n_1 \binom{n_0}{n_1} v^{n_0-n_1} w^{n_1} \\
&= 0 \cdot v^{n_0} + 1 \cdot [n_0] v^{n_0-1} w + 2 \cdot \left[\frac{n_0!}{2(n_0-2)!} \right] v^{n_0-2} w^2 + 3 \cdot \left[\frac{n_0!}{3!(n_0-3)!} \right] v^{n_0-3} w^3 + \cdots \\
&\quad + (n_0 - 1) \cdot \left[\frac{n_0!}{(n_0-1)!2} \right] v w^{n_0-1} + n_0 \cdot w^{n_0} \\
&= w \left\{ 0 \cdot v^{n_0} + 1 \cdot n_0 v^{n_0-1} + 2 \cdot \binom{n_0}{2} v^{n_0-2} w + 3 \cdot \binom{n_0}{3} v^{n_0-3} w^2 + \cdots \right. \\
&\quad \left. + (n_0-1) \cdot \binom{n_0}{n_0-1} v w^{n_0-2} + n_0 \cdot w^{n_0-1} \right\} \\
&= w \frac{\partial}{\partial w} \left\{ v^{n_0} + n_0 v^{n_0-1} w + \binom{n_0}{2} v^{n_0-2} w^2 + \cdots + \binom{n_0}{n_0-1} v w^{n_0-1} + w^{n_0} \right\} \\
&= w \frac{\partial}{\partial w} \left[\sum_{n_1=0}^{n_0} \binom{n_0}{n_1} v^{n_0-n_1} w^{n_1} \right] \\
&= w \frac{\partial}{\partial w} (v+w)^{n_0} \\
&= n_0 w (v+w)^{n_0-1} \\
&= n_0 w (1 - w + w)^{n_0-1} \\
&= n_0 w
\end{aligned} \tag{2.123}$$

Now $w(t)$ is derived in a similar way as above. Generalizing slightly Eq. (2.120), the general expression for the change in probability that a nucleus has not decayed is

$$dw = -\gamma(t) w dt, \qquad \text{such that} \qquad w(t) = \int_0^t e^{-\gamma(s)} ds. \tag{2.124}$$

With the more familiar assumption that γ is constant,

$$w(t) = e^{-\gamma t}, \tag{2.125}$$

such that

$$\langle N(t_1)\rangle = n_0 e^{-\gamma t}. \tag{2.126}$$

With this, the Markov process based on Eq. (2.122) becomes

$$P(n_1, t_1) = \binom{n_0}{n_1} e^{-n_1\gamma t_1}(1 - e^{-\gamma t_1})^{(n_0-n_1)} \tag{2.127}$$

$$P_{1|1}(n_2, t_2|n_1, t_1) = \binom{n_1}{n_2} e^{-n_2\gamma(t_2-t_1)}\left[1 - e^{-\gamma(t_2-t_1)}\right]^{(n_1-n_2)}, \tag{2.128}$$

where $n_1 - n_2$ is the number of nuclei that have decayed in time $t_2 - t_1$. Letting this time difference approach zero, $t_2 - t_1 \to 0$,

$$P_{1|1}(n_2, t_2|n_1, t_1) = \binom{n_1}{n_2} e^0[1 - e^0]^{(n_1-n_2)} = \delta_{n_1 n_2}, \tag{2.129}$$

where δ is the Kronecker delta. Now let $t_2 - t_1 = \tau$ and expand Eq. (2.128) in a Taylor series about $\tau = 0$:

$$\begin{aligned}
P_{1|1}(n_2, t_1 + \tau|n_1, t_1) &= \delta_{n_1 n_2} + \Bigg[-\gamma n_2 \binom{n_1}{n_2}\left(1 - e^{-\gamma\tau}\right)^{(n_1-n_2)} \\
&\quad + (n_1 - n_2)\binom{n_1}{n_2} e^{-n_2\gamma\tau}\left(1 - e^{-\gamma\tau}\right)^{(n_1-n_2-1)}\gamma e^{-\gamma\tau}\Bigg]_{\tau=0} \tau + O(\tau^2) \\
&= \delta_{n_1 n_2} - n_1\gamma\tau\delta_{n_1 n_2} + (n_1 - n_1 + 1)\binom{n_1}{n_1 - 1}\left[\left(1 - e^{-\gamma\tau}\right)^0 e^{-n_1\gamma\tau}\right]_{\tau=0}\gamma\tau + O(\tau^2) \\
&= \delta_{n_1 n_2} - n_1\gamma\tau\delta_{n_1 n_2} + \binom{n_1}{n_1 - 1}\delta_{n_1-1,n_2}\gamma\tau + O(\tau^2) \\
&= \delta_{n_1 n_2} - n_1\gamma\tau\delta_{n_1 n_2} + n_1\gamma\tau\delta_{n_1-1,n_2} + O(\tau^2) \\
&= \underbrace{(1 - n_1\gamma\tau)\ \delta_{n_1 n_2}}_{\substack{\text{probability that no} \\ \text{decay took place}}} + \underbrace{n_1\gamma\tau\ \delta_{n_1-1,n_2}}_{\substack{\text{probability that 1} \\ \text{nucleus decayed}}} + O(\tau^2)
\end{aligned} \tag{2.130}$$

A point that is not necessarily immediately obvious is that these two terms cannot be non-zero at the same time. If $n_2 = n_1$ then no decay took place, the first term is non-zero, and the delta function of the second term is zero. If $n_2 = n_1 - 1$, on the other hand, one nucleus has decayed, the first term is zero, and the second term is $n_1\gamma\tau$. This means that the probability is one or the other, their sum cannot happen. This is consistent with what we expect from the behaviour of a probability, as reflected in the product of probabilities of Eq. (2.129). Second, in this linear approximation of how the probability depends on the time interval, we see that if $\tau = 0$ then the probability is 1, as we also would expect. Third, for small τ, the equation allows for the contradictory condition that $n_2 = n_1$ at the same time only because it is an approximation. Finally, this approximation forces the introduction of a new concept: the factor $n_1\gamma$ necessarily becomes a *transition probability per unit time.*

2.3.3.6 The Master Equation

We can now look at what happens to $T_{\tau'}$ as $\tau' \to 0$. We can adapt Eq. (2.130) to a general homogeneous Markov process as

$$T_{\tau'}(y_2|y_1) = (1 - a_0\tau')\delta(y_2 - y_1) + \tau' W(y_2|y_1) + O(\tau'^2), \tag{2.131}$$

where $W(y_2|y_1)$ is the transition probability per unit time and $(1 - a_0\tau')$ is the probability that no transition takes place during τ'. Therefore,

$$a_0(y_2|y_1) = W(y_2|y_1), \qquad \text{so that} \qquad a_0(y_1) = \int W(y_2|y_1)dy_2. \tag{2.132}$$

$a_0(y_1)$ is the transition probability per unit time from state y_1 to state y_2, but integrated over all possible values of y_2.

The different treatment of the two terms in Eq. (2.131) (one is integrated and the other is not) is not a consequence of how a_0 is defined but, rather, of how the transition probability $T_{\tau'}(y_2|y_1)$ is defined. Referring to the basic definitions from earlier in this section, $T_{\tau'}(y_2|y_1)$ is the transition probability from a *specific* value of y_1 to any value of y_2. Thus, it is in essence a function of y_1. The definition of a_0 should therefore be seen as a consequence of this prior definition and interpretation of the transition probability.

Therefore, the transition probability for a small time interval τ' is given by the sum of two terms that cannot be non-zero at the same time, as for Eq. (2.130):

$$T_{\tau'}(y_2|y_1) = \left[1 - \tau' \int W(y_2|y_1)dy_2\right] \delta(y_2 - y_1) + \tau' W(y_2|y_1). \tag{2.133}$$

Now we can substitute this expression into the stationary process-version of the CKE, Eq. (2.116):

$$\begin{aligned} T_{\tau+\tau'}(y_3|y_1) &= \int T_{\tau'}(y_3|y_2)T_\tau(y_2|y_1)dy_2 \\ &= \int \Big\{ \left[1 - \tau' a_0(y_2)\right] \delta(y_3 - y_2) + \tau' W(y_3|y_2) \Big\} T_\tau(y_2|y_1)dy_2 \end{aligned} \tag{2.134}$$

Note that in this equation $a_0(y_2)$ is the transition probability between state y_2 and state y_3 integrated over all possible values of y_3. Hence, the first term is the probability that the transition $2 \to 3$ did not happen. Continuing with the elaboration,

$$\begin{aligned} T_{\tau+\tau'}(y_3|y_1) &= \int \left[1 - \tau' a_0(y_2)\right] \delta(y_3 - y_2)T_\tau(y_2|y_1)dy_2 + \tau' \int W(y_3|y_2)T_\tau(y_2|y_1)dy_2 \\ &= \left[1 - \tau' a_0(y_3)\right] T_\tau(y_3|y_1) + \tau' \int W(y_3|y_2)T_\tau(y_2|y_1)dy_2, \end{aligned} \tag{2.135}$$

where in the last step we have used the delta function rule for integration. The second term of Eq. (2.135) is now the probability of transition from state 2 to state 3 times the probability that the system has arrived in state 2 (from state 1). The first term is much trickier, mainly because of $a_0(y_3)$. The nature of the delta function when integrated is such that a_0 is genuinely a function of y_3, because the only non-zero term in the integrand that could be retained was when $y_2 = y_3$. However, it is not clear which other variable was integrated in order to obtain this function (see Eq. (2.132)). Mathematically, y_1 is just as legitimate a choice as y_2. However, if we choose y_1 the resulting equation is not as useful. Therefore, let's choose y_2 and proceed. Namely, now we divide by τ' and let $\tau' \to 0$:

$$\begin{aligned} \lim_{\tau'\to 0}\left[\frac{T_{\tau+\tau'}(y_3|y_1)}{\tau'}\right] &= \lim_{\tau'\to 0}\left[\frac{T_\tau(y_3|y_1)}{\tau'}\right] - a_0(y_3)T_\tau(y_3|y_1) + \int W(y_3|y_2)T_\tau(y_2|y_1)dy_2 \\ \lim_{\tau'\to 0}\left[\frac{T_{\tau+\tau'}(y_3|y_1) - T_\tau(y_3|y_1)}{\tau'}\right] &= -\left[\int W(y_2|y_3)dy_2\right] T_\tau(y_3|y_1) + \int W(y_3|y_2)T_\tau(y_2|y_1)dy_2 \\ \frac{\partial}{\partial \tau}T_\tau(y_3|y_1) &= \int \left[W(y_3|y_2)T_\tau(y_2|y_1) - W(y_2|y_3)T_\tau(y_3|y_1)\right] dy_2, \end{aligned}$$

where in the last equation we have switched the order of the terms on the RHS and moved $T_\tau(y_3|y_1)$ under the integral sign since it does not involve y_2. So the new term, which is now the second one, is the probability of transition from state 3 to state 2 times the probability that the system has arrived in state 3 (from state 1). The fact that both states 2 and 3 came from the same state 1 allows us to treat it as arbitrary. Thus, letting now $y = y_3$ and $y' = y_2$, we obtain the continuous Master equation:

$$\frac{\partial P(y,t)}{\partial t} = \int \left[W(y|y')P(y',t) - W(y'|y)P(y,t)\right] dy'. \tag{2.136}$$

This PDE is an equation for the *transition* probability. Take t_1 and y_1 and look at the solution for $t \geq t_1$, with initial condition

$$P(y_1, t_1) = \delta(t - t_1). \tag{2.137}$$

The solution is the transition probability $T_{t-t_1}(y|y_1)$ of the Markov process. The discrete form of this equation is perhaps easier to understand and to relate to BIOMICS:

$$\boxed{\frac{dP_n(t)}{dt} = \sum_{n'} \left[W_{nn'} P_{n'}(t) - W_{n'n} P_n(t) \right].} \tag{2.138}$$

In this formulation, it is natural to interpret the possible (discrete) values of the stochastic variable as abstract states of some (finite-state) automaton. Let us assume that we have a probabilistic automaton with N states. Then the transition probability of state $n \in \{1, \cdots, N\}$ is given by the sum of all possible probability flux balances between that state n and all the other states n' of the automaton. Each member of the sum in Eq. (2.138) contributes to the time rate of change of the transition probability of state n. For each member of the sum, the first term is the transition probability *per unit time* from state n' **into** state n, weighted by the probability that the automaton is in state n'. The second term, on the other hand, is the opposite: the transition probability *per unit time* from state n **out to** state n', weighted by the probability that the automaton is in state n. Because the Ws are probabilities per unit time, they are really probability fluxes. Therefore, the Master equation is none other than a 'conservation of probability' equation, analogous to the conservation of mass equation of fluid mechanics.

The relevance to BIOMICS stems from the fact that the modelling of the (meta)stability properties of dynamical systems from biology appears to be more easily achieved through a stochastic approach than through an exact analytical solution. This equation shows that the transition probabilities between states as dictated by the stochastic model are related to analogous transitions between states.

One rather difficult and abstract point, however, remains to be addressed. We said that the original CKE (2.116) was a probabilistic version of the closure condition for semigroups. How has this condition been changed by this derivation? In other words, does the Master equation still embody this condition? The closure condition says that the transition probability from 1 to 3 is the product between the transition probability between 1 to 2 and 2 to 3, integrated over all possible values of the probability that the system is in state 2. Thus, intuitively the Master equation is an infinitesimal version of this statement centred on state 2: the time rate of change of the probability of state 2 is the flux balance between the probability into and out of 2. That the algebraic closure condition for groups and semigroups should correspond to a conservation equation of the same form for mass and probability is very interesting and warrants further study beyond the end of BIOMICS.

The Master equation is the first step in the derivation of the quasi-potential function. To be sure, it is not strictly needed from the point of view of the algebraic aspects of the derivation, but it is helpful for providing a reference basis for stochastic modelling. For example, the next step in this foundation-building process is to derive the Fokker-Planck equation. The Fokker-Planck equation can be seen as a Taylor expansion of the Master equation to second order in terms of the size of the probabilistic state transitions, and in particular for *small* transitions [46]. As discussed in [46], it represents a model of Brownian motion that is mathematically equivalent to the Langevin equation, which is based on very different starting assumptions: Newton's law in the presence of a deterministic drift force field and a fluctuating force rather than probabilistic transitions of an abstract stochastic variable. But also Langevin's equation is dependent on the magnitude of the fluctuating force being small relative to the drift force field.

These considerations are meant as an aid for further study, a roadmap to connect mathematically different areas of physical and biological science underpinning the meta-stable behaviour of dynamical systems, towards the development of a more general theory of their dynamical stability. What is left for the purposes of this report is a summary of the concepts underlying the quasi-potential. For this we need the Smoluchowski-Kramers approximation to the Langevin equation, already discussed above, within the context of Freidlin and Wentzell's [18] theory of large deviations.

2.4 The Quasi-Potential of Meta-Stable Dynamical Systems

Freidlin and Wentzell's [18] theory of large deviations concerns stochastic meta-stable processes governed by a potential. As discussed in [23], because the fluctuating or noise component of the force is small, such systems will spend an overwhelming proportion of time near a given local minimum, and only very rarely will they exhibit large oscillations capable of moving them to a different meta-stable state. This is referred to as the 'exit problem', meaning exit from a domain defined by the basin of attraction of a given meta-stable state. When, after a sufficiently long time, the system does exit a given attraction basin, Freidlin and Wentzell's [18] theory shows that the path followed by such 'large deviations' will be close to the Least Action Path (LAP) with overwhelming probability.

More precisely, for small Gaussian noise the asymptotics of the probability of large deviations are of the form $e^{-C\epsilon^{-2}}$ as $\epsilon \to 0$, where C is a constant and ϵ is a small parameter [18]. It turns out we can introduce a functional $S(\phi)$ defined on smooth functions (smoother than the trajectories $X^\epsilon(t)$ of the perturbed system) such that

$$P\{\rho(X^\epsilon, \phi) < \delta\} \approx e^{-S(\phi)\epsilon^{-2}} = \frac{1}{e^{\frac{S(\phi)}{\epsilon^2}}}, \tag{2.139}$$

where $P\{\cdot\}$ indicate the probability of its argument, $\rho(\cdot, \cdot)$ is a distance function in some function space, and δ is a small positive number. The probability of an unlikely event is distributed over contributions of the form above corresponding to different paths $\phi(t)$. Therefore, the most likely will be those for which $S(\phi)$ is minimum.

Freidlin and Wentzell define the action functional by analogy with Feynman's action integral of the quantum mechanical paths. As Planck's constant $\hbar \to 0$ the quantum mechanical paths converge to the classical mechanical paths consistent with Hamilton's principle. The small parameter ϵ of stochastic perturbation is treated in a similar way. The action functional is therefore first defined for a pure Wiener process where the drift force term is identically zero (note this is not an ODE),

$$X^\epsilon = \epsilon w, \tag{2.140}$$

as

$$S(\phi) = \frac{1}{2}\int_0^T |\dot{w}|^2 \, dt. \tag{2.141}$$

Of the several kinds of random processes discussed by Freidlin and Wentzell we focus on Wiener processes, which correspond to Brownian motion and whose Fourier transform has a slope of -2 on a log-log plot. This implies a strong autocorrelation and therefore a relatively high predictability, which is consistent with the assumption of small noise relative to the deterministic motion. Thus, we are within the scope of the Langevin equation and its Smoluchowski-Kramers approximation (2.96), which we rewrite in the simpler form

$$\dot{q} = b(q) + \epsilon\dot{w}. \tag{2.142}$$

The system's LAP from a given point is none other than the minimizer of a generalization of Hamilton's action that is based on the fluctuating component:

$$S_T = \frac{1}{2}\int_0^T |\dot{q} - b(q)|^2 \, dt, \tag{2.143}$$

where we refer the reader to Freidlin and Wentzell's lengthy and rigorous derivations for the treatment of ϵ as a normalizing factor.

As discussed by [9], determination of the action is easier when the system is governed by a gradient drift force field, i.e. a force field $b(q) = -\nabla V$, where $V(q)$ is a potential function:[17]

$$\begin{aligned} S_T &= \frac{1}{2} \int_0^T |\dot{q} + \nabla V|^2 \, dt \\ &= \frac{1}{2} \int_0^T \left[|\dot{q} - \nabla V|^2 + 4(\nabla V \cdot \dot{q}) \right] dt. \end{aligned} \tag{2.144}$$

The minimum of this integral will obtain when the state trajectory $q(t)$ is everywhere parallel to the gradient of the potential V since in this case the only contribution will be from the noise term. We can arrive at a useful inequality by focusing on the corresponding deterministic system, i.e. the system in which the noise is zero. For such system, the first term in the integral necessarily vanishes, such that:

$$S_T \geq 2(V(T) - V_0). \tag{2.145}$$

We note that this result follows from the chain rule since integration of the second term w.r.t. time is equivalent to a line integral of the gradient of a potential, which yields the difference in its values at the end-points.

[51]

[17] We should recall that since we are now talking about 1st-order systems of ODE modelling biochemical reactions, phase space and configuration space are one and the same.

Chapter 3

Ordinary differential equations of order m having a given symmetry group of dimension r for $m > r - 2$

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Abstract

Here we present Lie's method to find ordinary differential equations of order m allowing a given Lie group of dimension r as a group of their symmetries where $m > r - 2$. We illustrate this method with several examples.

3.1 Introduction

Lie has determined the groups of transformations of the (x, y)-plane and put these into canonical form (cf. [32, Sections 3, 4, 5, p. 28–78], and in [32, Section 19 , p. 360–392],). In [33, Section X, p. 243–248], he has given a method to find the ordinary differential equations which admit a given Lie group as a group of their symmetries. In [33, Sections X, XI, XIV, XVI], he provided a classification of all ordinary differential equations of arbitrary order admitting these given groups as groups of their symmetries. In [17, Chapter 4] we have considered Lie's method and classified ordinary differential equations admitting some of these symmetry groups in the case where the order m and the dimension r has $m \leq r - 2$. In Section 3.2 we introduce Lie's method for the case $m > r - 2$, then apply it to some examples in Section 3.3. First, we review the method for $m \leq r - 2$ (cf. [17, Chapter 4]).

Let X_i, $i = 1, 2, \ldots, r$, be the infinitesimal generators of the tangential Lie algebra $\mathbf{g}$ of a given r-dimensional real Lie group G. Then one has

$$X_i = \phi_i(x, y) \frac{\partial}{\partial x} + \eta_i(x, y) \frac{\partial}{\partial y}, \ i = 1, 2, \ldots, r \tag{3.1}$$

for some smooth functions $\phi_i, \eta_i \colon \mathbb{R}^2 \to \mathbb{R}$. The m-th prolonged vector fields $X_i^{(m)}$, $i = 1, 2, \ldots, r$, are defined as

$$X_i^{(m)} = \phi_i(x, y) \frac{\partial}{\partial x} + \eta_i(x, y) \frac{\partial}{\partial y} + \eta_i^{(1)}(x, y, y') \frac{\partial}{\partial y'} + \cdots + \eta_i^{(m)}\left(x, y, y', \ldots, y^{(m)}\right) \frac{\partial}{\partial y^{(m)}}, \tag{3.2}$$

where $\eta_i^{(k)}$, $k = 1, 2, ..., m$, is the k-th coordinate function of the prolongation of the vector field X_i, and $y^{(k)}$ denotes the kth derivative of y with respect to x. The functions $\eta_i^{(k)}$ can be computed recursively as

$$\eta_i^{(k)} = \frac{d\eta_i^{(k-1)}}{dx} - y^{(k)} \frac{d\phi_i}{dx},$$

where d/dx denotes the *total derivative* with respect to x (cf. [33, Section X, p. 245]). Note, that partial derivative by x is denoted by $\partial/\partial x$. The exact formulas can be found in e.g. [17, Section 4.2, p. 48]. The vector fields $X_i^{(m)}$, $i = 1, 2, \ldots, r$, depend on x, y, y', $\ldots$, $y^{(m)}$, and they generate a Lie algebra isomorphic to $\mathbf{g}$ (cf. [33, Section X, p. 245]). A differential equation

$$f\left(x, y, y', \ldots, y^{(m)}\right) = 0$$

of order m admits a group of symmetries whose tangential Lie algebra is $\mathbf{g}$ if and only if the system of partial differential equations

$$X_1^{(m)} f = X_2^{(m)} f = \cdots = X_i^{(m)} f = \cdots = X_r^{(m)} f = 0$$

is satisfied whenever $f\left(x, y, y', \ldots, y^{(m)}\right) = 0$ holds. That is, if and only if

$$\begin{aligned}
\phi_1 \frac{\partial f}{\partial x} + \eta_1 \frac{\partial f}{\partial y} + \eta_1^{(1)} \frac{\partial f}{\partial y'} + \cdots + \eta_1^{(m)} \frac{\partial f}{\partial y^{(m)}} &= 0, \\
\phi_2 \frac{\partial f}{\partial x} + \eta_2 \frac{\partial f}{\partial y} + \eta_2^{(1)} \frac{\partial f}{\partial y'} + \cdots + \eta_2^{(m)} \frac{\partial f}{\partial y^{(m)}} &= 0, \\
&\vdots \\
\phi_i \frac{\partial f}{\partial x} + \eta_i \frac{\partial f}{\partial y} + \eta_i^{(1)} \frac{\partial f}{\partial y'} + \cdots + \eta_i^{(m)} \frac{\partial f}{\partial y^{(m)}} &= 0, \\
&\vdots \\
\phi_r \frac{\partial f}{\partial x} + \eta_r \frac{\partial f}{\partial y} + \eta_r^{(1)} \frac{\partial f}{\partial y'} + \cdots + \eta_r^{(m)} \frac{\partial f}{\partial y^{(m)}} &= 0
\end{aligned} \tag{3.3}$$

is satisfied whenever $f\left(x, y, y', \ldots, y^{(m)}\right) = 0$ holds. If $m \leq r-2$, then the method of Lie says the following.

Theorem 1 ([17, Theorem 4.1]))**.** *To find the differential equations $f\left(x, y, y', ..., y^{(m)}\right) = 0$ of order m admitting a group of symmetries whose tangential Lie algebra is a given r-dimensional real Lie algebra $\mathbf{g}$ such that $m \leq r-2$, one has to build the matrix*

$$M = \begin{pmatrix} \phi_1 & \phi_2 & \phi_3 & \cdots & \phi_r \\ \eta_1 & \eta_2 & \eta_3 & \cdots & \eta_r \\ \eta_1^{(1)} & \eta_2^{(1)} & \eta_3^{(1)} & \cdots & \eta_r^{(1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \eta_1^{(m)} & \eta_2^{(m)} & \eta_3^{(m)} & \cdots & \eta_r^{(m)} \end{pmatrix}, \tag{3.4}$$

and compute the greatest common divisor of all $(m+2) \times (m+2)$ subdeterminants. The factors of this polynomial give the only possibilities for the sought differential equations, unless this polynomial is identically 0*.*

If $m > r-2$ then one has to solve the system of the partial differential equations given by (3.3) to obtain the differential equations of order m which allow the group of symmetries corresponding to the Lie algebra $\mathbf{g}$. This problem is equivalent to computing the independent invariants for the r-dimensional Lie group of transformations G (cf. [40, Chapter 2]). This computation can get very complicated when $r > 1$. We explain this method in Section 3.2 and illustrate the computations with examples in Section 3.3.

3.2 Lie's method to find the ordinary differential equations of order m having a given symmetry group of dimension r for $m > r-2$

In this section we present the method of Lie to obtain the ordinary differential equations of order m which allow a given Lie group G of dimension r as the group of their symmetries for $m > r-2$. This method can be found in [33, p. 247–248].

Suppose that G is an r-dimensional Lie group of transformations acting on $M \subset \mathbb{R}^2$ such that the tangential Lie algebra $\mathbf{g}$ of G is given by the infinitesimal generators (3.1). We consider the m-th prolongation $G^{(m)}$ of G, its tangential Lie algebra is given by the vector field in (3.2). Assume

$m > r-2$. Now, $G^{(m)}$ acts on the $(m+2)$-dimensional manifold $M^{(m)} = \{x, y, y', \dots, y^{(m)}\}$. Assume that the top-left $r \times r$ subdeterminant of M given by (3.4) is not identically zero. Then the system of the partial differential equations given by (3.3) is complete with $m+2-r$ common solutions. If $m+2 = r+1$ then there exists a solution φ_1 of (3.3) which can be found by integration. The solution φ_1 depends solely on the variables $x, y, y', \dots, y^{(r-1)}$. If $m+2 = r+2$ then there are two solutions of (3.3). One is φ_1, the other is φ_2 which depends on the variables $x, y, y', \dots, y^{(r)}$. If $m+2 = r+3$ then there are three solutions φ_i, $i = 1, 2, 3$, such that φ_3 depends on x, y, $y', \dots, y^{(r+1)}$, etc. For arbitrary m there are $m-r+2$ solutions φ_j, $j = 1, 2, \dots, m-r+2$. Now we show that it is enough to determine the solutions φ_1, φ_2 by integration.

If we know the solutions φ_1, φ_2, then for all $i \geq 3$ the solutions φ_i can be found using φ_1 and φ_2 by differentiation in the following way. The equation

$$\varphi_2 - a\varphi_1 + b = 0$$

with arbitrary constants a, b is a differential equation of order r which is invariant under the action of $\mathbf{g}$. Indeed, for any $X_i^{(m)}$ in (3.2) we have

$$X_i^{(m)} (\varphi_2 - a\varphi_1 + b) = 0,$$

if φ_1 and φ_2 are solutions of (3.3). By differentiation of this equation with respect to the variable x one obtains

$$\begin{aligned} &\frac{d\phi_i}{dx}\left(\frac{\partial(\varphi_2 - a\varphi_1 + b)}{\partial x}\right) + \phi_i \frac{d}{dx}\left(\frac{\partial \varphi_2}{\partial x} - a\frac{\partial \varphi_1}{\partial x}\right) \\ &+\frac{d\eta_i}{dx}\left(\frac{\partial(\varphi_2 - a\varphi_1 + b)}{\partial y}\right) + \eta_i \frac{d}{dx}\left(\frac{\partial \varphi_2}{\partial y} - a\frac{\partial \varphi_1}{\partial y}\right) \\ &+\frac{d\eta_i^{(1)}}{dx}\left(\frac{\partial(\varphi_2 - a\varphi_1 + b)}{\partial y'}\right) + \eta_i^{(1)} \frac{d}{dx}\left(\frac{\partial \varphi_2}{\partial y'} - a\frac{\partial \varphi_1}{\partial y'}\right) \\ &+\cdots \\ &+\frac{d\eta_i^{(m)}}{dx}\left(\frac{\partial(\varphi_2 - a\varphi_1 + b)}{\partial y^{(m)}}\right) + \phi_i^{(m)} \frac{d}{dx}\left(\frac{\partial \varphi_2}{\partial y^{(m)}} - a\frac{\partial \varphi_1}{\partial y^{(m)}}\right). \end{aligned} \tag{3.5}$$

Now, using $\varphi_2 - a\varphi_1 + b = 0$, the first term of every line in (3.5) cancels. Thus, we obtain

$$X_i^{(m)} \frac{d}{dx} (\varphi_2 - a\varphi_1) = 0,$$

and therefore the differential equation

$$\frac{d\varphi_2}{dx} - a\frac{d\varphi_1}{dx} = 0,$$

or equivalently

$$\frac{\frac{d\varphi_2}{dx}}{\frac{d\varphi_1}{dx}} = a. \tag{3.6}$$

Now, (3.6) is a differential equation of order $r+1$ which is invariant under the action of $\mathbf{g}$. Hence one can choose $\frac{d\varphi_2}{dx} / \frac{d\varphi_1}{dx}$ as φ_3. This φ_3 is functionally independent of φ_1 and φ_2, because φ_1 and φ_2 do not depend on $y^{(r+1)}$, but φ_3 does. Further, in a similar manner it can be shown that $\frac{d\varphi_3}{dx} / \frac{d\varphi_1}{dx}$ can be chosen as φ_4, etc.

Theorem 2 ([33, p. 247–248])**.** *Any differential equation of order $m > r+2$ which admit a group of symmetries whose tangential Lie algebra is a given r-dimensional real Lie algebra $\mathbf{g}$ given by*

$$X_i = \phi_i(x, y)\frac{\partial}{\partial x} + \eta_i(x, y)\frac{\partial}{\partial y}, \ \ i = 1, 2, \dots, r,$$

has the form

$$\Omega(\varphi_1, \varphi_2, \varphi_3, \dots) = 0,$$

with some smooth function Ω.

For the concrete calculations of differential equations of order $m > r+2$ admitting the symmetry group whose tangential Lie algebra is given by the vector fields X_i, $i = 1, 2, \ldots, r$, we proceed in the following way.

1. We have to find two common solutions φ_1, φ_2 of the system of partial differential equations given by (3.30) with $m = r$ such that φ_1 is a function of $x, y, \ldots, y^{(r-1)}$ and φ_2 is a function of $x, y, \ldots, y^{(r)}$. For this, we first compute the $(r-1)$th and rth prolonged vector fields $X_i^{(r-1)}$, $X_i^{(r)}$, $i = 1, 2, \ldots, r$.
2. We determine the joint invariants of all the $(r-1)$th prolonged vector fields $X_i^{(r-1)}$, $i = 1, 2, \ldots, r$. To obtain these we determine by integration the functionally independent invariants $\alpha_j\left(x, y, ..., y^{(r-1)}\right)$ of one of the vector fields, say $X_1^{(r-1)}$. These invariants are the solutions of the linear homogeneous partial differential equation
$$X_1^{(r-1)}(\alpha) = \phi_1 \frac{\partial \alpha}{\partial x} + \eta_1 \frac{\partial \alpha}{\partial y} + \eta_1^{(1)} \frac{\partial \alpha}{\partial y'} + \cdots + \eta_1^{(r-1)} \frac{\partial \alpha}{\partial y^{(r-1)}} = 0. \tag{3.7}$$
If $X_1(\alpha) \neq 0$ in a neighbourhood of a chosen point x_0, then there are $r+1$ functionally independent invariants, hence $r+1$ functionally independent solutions of the partial differential equation (3.7) in a neighbourhood of x_0.
3. Since any joint invariant φ must in particular be an invariant of $X_1^{(r-1)}$, we can write φ as some function of the computed invariants α_j, $j = 1, 2, ..., r+1$, of $X_1^{(r-1)}$. Using the invariants α_j, $j = 1, 2, ..., r+1$, of $X_1^{(r-1)}$ as new variables (coordinates), we express the remaining vector fields $X_2^{(r-1)}, \ldots, X_r^{(r-1)}$ in these new coordinates. Then we find joint invariants of these *new* $r-1$ vector fields $X_2^{(r-1)}(\alpha_j), \ldots, X_r^{(r-1)}(\alpha_j)$. This procedure works inductively leading eventually to all of the vector fields expressed in terms of the joint invariants of α_j, $j = 1, 2, ..., r+1$. This gives $\varphi_1 = \Psi_1(\alpha_1, \alpha_2, ..., \alpha_{r+1})$.
4. Then we determine the joint invariants of all the rth prolonged vector fields $X_i^{(r)}$, $i = 1, 2, \ldots, r$. One is φ_1. To obtain the other one we proceed in the same way as in items 2 and 3. First we determine by integration the functionally independent invariants $\beta_1, \beta_2, \ldots, \beta_{r+1}$, of one of the vector fields, say $X_1^{(r)}$. Applying item 3, we obtain step by step the joint invariants of all the rth prolonged vector fields expressed in terms of the joint invariants of the first β_j, $j = 1, 2, ..., r+1$, of them. Denote by K the subset of $\{1, 2, ..., r+1\}$ consisting of those indices k such that the invariant β_k does not depend on the variable $y^{(r)}$. The invariant φ_1 is a smooth function of these invariants β_k, $k \in K$. Therefore one has $\varphi_2 = \Psi_2(\varphi_1, \beta_l, ...)$, where $l \in \{1, 2, ..., r+1\} \setminus K$, as these are the indices of the invariants which depend on $y^{(r)}$.
5. We obtain the further common solutions φ_i, $i = 3, 4, \ldots,$ of (3.3) for arbitrary m by the rule $\varphi_i = \frac{d\varphi_{i-1}}{dx} / \frac{d\varphi_1}{dx}$.

3.3 Examples

Applying the method of Section 3.2 we give examples of ordinary differential equations of order m allowing a given Lie symmetry group of dimension r such that $m > r - 2$.

Example 1. The Lie algebra $\mathbf{g_1} = \mathbf{sl_2}(\mathbb{R})$ is generated by the vector fields
$$X_1 = \frac{\partial}{\partial x} + \frac{\partial}{\partial y}, \qquad X_2 = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}, \qquad X_3 = x^2\frac{\partial}{\partial x} + y^2\frac{\partial}{\partial y}. \tag{3.8}$$
By [17, Example 4.4] there is precisely one differential equation $y' = 0$ of order one which is invariant under the group of symmetries corresponding to the Lie algebra $\mathbf{g}_1$.

To determine all ordinary differential equations of order $m \geq 2$ which are invariant under the 3-dimensional group of symmetries corresponding to the Lie algebra $\mathbf{g}_1$ we need to compute the 3rd prolonged vector fields $X_i^{(3)}$ of (3.8). Using
$$(\phi_1, \phi_2, \phi_3) = \left(1, x, x^2\right), \qquad (\eta_1, \eta_2, \eta_3) = \left(1, y, y^2\right), \tag{3.9}$$

we obtain

$$\left(\eta_1^{(1)}, \eta_2^{(1)}, \eta_3^{(1)}\right) = \left(0, 0, \left(2y - 2x\right) y'\right), \tag{3.10}$$

$$\left(\eta_1^{(2)}, \eta_2^{(2)}, \eta_3^{(2)}\right) = \left(0, -y^{(2)}, -2y' + 2\left(y'\right)^2 - 4xy^{(2)} + 2yy^{(2)}\right), \tag{3.11}$$

$$\left(\eta_1^{(3)}, \eta_2^{(3)}, \eta_3^{(3)}\right) = \left(0, -2y^{(3)}, -6y^{(2)} + 6y^{(2)}y' - 6xy^{(3)} + 2yy^{(3)}\right). \tag{3.12}$$

This yields the following system of partial differential equations

$$\begin{aligned} \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} &= 0, \\ x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} - y^{(2)}\frac{\partial f}{\partial y^{(2)}} - 2y^{(3)}\frac{\partial f}{\partial y^{(3)}} &= 0, \\ x^2\frac{\partial f}{\partial x} + y^2\frac{\partial f}{\partial y} + 2\left(y - x\right)y'\frac{\partial f}{\partial y'} + 2\left(yy^{(2)} - 2xy^{(2)} + \left(y'\right)^2 - y'\right)\frac{\partial f}{\partial y^{(2)}} & \\ +2\left(yy^{(3)} - 3xy^{(3)} - 3y^{(2)} + 3y^{(2)}y'\right)\frac{\partial f}{\partial y^{(3)}} &= 0. \end{aligned} \tag{3.13}$$

From the first equation of (3.13) it follows that f depends on $x - y$. Using this the second and third equation reduce to

$$\begin{aligned} \left(y - x\right)\frac{\partial f}{\partial y} - y^{(2)}\frac{\partial f}{\partial y^{(2)}} - 2y^{(3)}\frac{\partial f}{\partial y^{(3)}} &= 0, \\ 2\left(y - x\right)y'\frac{\partial f}{\partial y'} + \left(2\left(y'\right)^2 - 2y' + 3\left(y - x\right)y^{(2)}\right)\frac{\partial f}{\partial y^{(2)}} & \\ + \left(6y^{(2)}y' - 6y^{(2)} + 4\left(y - x\right)y^{(3)}\right)\frac{\partial f}{\partial y^{(3)}} &= 0. \end{aligned} \tag{3.14}$$

By integration of the first equation of (3.14) we obtain that its solutions are generated by

$$y', \qquad \alpha = \left(y - x\right)y^{(2)}, \qquad \beta = \left(y - x\right)^2 y^{(3)}. \tag{3.15}$$

Taking these as new variables, the vector field corresponding to the left-hand side of the second equation of (3.14)

$$Y = 2\left(y - x\right)y'\frac{\partial}{\partial y'} + \left(2y'\left(y' - 1\right) + 3\left(y - x\right)y^{(2)}\right)\frac{\partial}{\partial y^{(2)}} + \left(6y^{(2)}\left(y' - 1\right) + 4\left(y - x\right)y^{(3)}\right)\frac{\partial}{\partial y^{(3)}}$$

takes the form

$$\widetilde{Y} = 2y'\frac{\partial}{\partial y'} + \left(3\alpha + 2\left(y'\right)^2 - 2y'\right)\frac{\partial}{\partial \alpha} + \left(4\beta + 6\alpha\left(y' - 1\right)\right)\frac{\partial}{\partial \beta}. \tag{3.16}$$

The solutions of the partial differential equation

$$2y'\frac{\partial f}{\partial y'} + \left(3\alpha + 2\left(y'\right)^2 - 2y'\right)\frac{\partial f}{\partial \alpha} + \left(4\beta + 6\alpha\left(y' - 1\right)\right)\frac{\partial f}{\partial \beta} = 0$$

are generated by

$$\varphi_1 = \alpha\left(y'\right)^{-\frac{3}{2}} - 2\left(\left(y'\right)^{\frac{1}{2}} + \left(y'\right)^{-\frac{1}{2}}\right) = \left(y - x\right)y^{(2)}\left(y'\right)^{-\frac{3}{2}} - 2\left(\left(y'\right)^{\frac{1}{2}} + \left(y'\right)^{-\frac{1}{2}}\right), \tag{3.17}$$

$$\begin{aligned} \varphi_2 &= \beta\left(y'\right)^{-2} - 6\varphi_1\left(\left(y'\right)^{\frac{1}{2}} + \left(y'\right)^{-\frac{1}{2}}\right) - 6\left(y' + \left(y'\right)^{-1}\right) \\ &= \left(y - x\right)^2 y^{(3)}\left(y'\right)^{-2} - 6\left(y - x\right)y^{(2)}\left(\left(y'\right)^{-2} + \left(y'\right)^{-1}\right) + 18y' + 24 + 18\left(y'\right)^{-1}. \end{aligned} \tag{3.18}$$

According to Theorem 2 the ordinary differential equations of order $m \geq 2$ which are invariant under the 3-dimensional group of symmetries corresponding to the Lie algebra $\mathbf{g}_1$ have the form

$$\Omega\left(\varphi_1, \varphi_2, \varphi_3, \dots\right) = 0,$$

where φ_1, φ_2 have the form (3.17), (3.18) and for $i = 3, 4, \ldots$ one has $\varphi_i = \frac{d\varphi_{i-1}}{dx} / \frac{d\varphi_1}{dx}$, and Ω is an arbitrary function.

Example 2. The Lie algebra $\mathbf{g_2} = \mathbf{sl_2}(\mathbb{R})$ is generated by the vector fields

$$X_1 = \frac{\partial}{\partial x}, \qquad X_2 = 2x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}, \qquad X_3 = x^2\frac{\partial}{\partial x} + xy\frac{\partial}{\partial y}. \tag{3.19}$$

By [17, Example 4.5] there does not exist any first order ordinary differential equation which is invariant under the group of symmetries corresponding to the Lie algebra $\mathbf{g}_2$.

To determine all ordinary differential equations of order $m \geq 2$ which are invariant under the 3-dimensional group of symmetries corresponding to the Lie algebra $\mathbf{g}_2$ we need to compute the 3rd prolonged vector fields $X_i^{(3)}$ of (3.19). As one has

$$(\phi_1, \phi_2, \phi_3) = \left(1, 2x, x^2\right), \qquad (\eta_1, \eta_2, \eta_3) = (0, y, xy),$$

we obtain

$$\begin{aligned}
\left(\eta_1^{(1)}, \eta_2^{(1)}, \eta_3^{(1)}\right) &= \left(0, -y', y - xy'\right), \\
\left(\eta_1^{(2)}, \eta_2^{(2)}, \eta_3^{(2)}\right) &= \left(0, -3y^{(2)}, -3xy^{(2)}\right), \\
\left(\eta_1^{(3)}, \eta_2^{(3)}, \eta_3^{(3)}\right) &= \left(0, -5y^{(3)}, -3y^{(2)} - 5xy^{(3)}\right).
\end{aligned}$$

Therefore we have to solve the system of partial differential equations

$$\begin{aligned}
\frac{\partial f}{\partial x} &= 0, \\
2x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} - y'\frac{\partial f}{\partial y'} - 3y^{(2)}\frac{\partial f}{\partial y^{(2)}} - 5y^{(3)}\frac{\partial f}{\partial y^{(3)}} &= 0, \\
x^2\frac{\partial f}{\partial x} + xy\frac{\partial f}{\partial y} + \left(y - xy'\right)\frac{\partial f}{\partial y'} - 3xy^{(2)}\frac{\partial f}{\partial y^{(2)}} - \left(3y^{(2)} + 5xy^{(3)}\right)\frac{\partial f}{\partial y^{(3)}} &= 0.
\end{aligned} \tag{3.20}$$

From the first equation of (3.20) it follows that f does not depend on the variable x. Using this, system (3.20) reduces to

$$\begin{aligned}
y\frac{\partial f}{\partial y} - y'\frac{\partial f}{\partial y'} - 3y^{(2)}\frac{\partial f}{\partial y^{(2)}} - 5y^{(3)}\frac{\partial f}{\partial y^{(3)}} &= 0, \\
y\frac{\partial f}{\partial y'} - 3y^{(2)}\frac{\partial f}{\partial y^{(3)}} &= 0.
\end{aligned} \tag{3.21}$$

The solutions of the second equation of (3.21) are generated by

$$y, \qquad y^{(2)}, \qquad \beta = \frac{3y^{(2)}y'}{y} + y^{(3)}. \tag{3.22}$$

Taking the functions in (3.22) as new variables, the vector field $Y = y\frac{\partial f}{\partial y} - y'\frac{\partial f}{\partial y'} - 3y^{(2)}\frac{\partial f}{\partial y^{(2)}} - 5y^{(3)}\frac{\partial f}{\partial y^{(3)}}$ can be written into the form

$$\widetilde{Y} = Y(y)\frac{\partial}{\partial y} + Y\left(y^{(2)}\right)\frac{\partial}{\partial y^{(2)}} + Y(\beta)\frac{\partial}{\partial \beta} = y\frac{\partial}{\partial y} - 3y^{(2)}\frac{\partial}{\partial y^{(2)}} - 5\beta\frac{\partial}{\partial \beta}.$$

Using integration, the solutions of the partial differential equation

$$y\frac{\partial f}{\partial y} - 3y^{(2)}\frac{\partial f}{\partial y^{(2)}} - 5\beta\frac{\partial f}{\partial \beta} = 0$$

are generated by

$$\varphi_1 = y^3y^{(2)}, \qquad \varphi_2 = \beta y^5 = y^4\left(3y^{(2)}y' + y^{(3)}y\right). \tag{3.23}$$

According to Theorem 2 any ordinary differential equation of order $m \geq 2$ which is invariant under the action of $\mathbf{g}_2$ has the form

$$\Omega(\varphi_1, \varphi_2, \varphi_3, \dots) = 0,$$

where φ_1, φ_2 are given by (3.23), and Ω is an arbitrary function.

Example 3. The Lie algebra $\mathbf{g}_3 = \mathbf{sl_2}(\mathbb{R})$ is generated by the vector fields

$$X_1 = \frac{\partial}{\partial y}, \qquad X_2 = y\frac{\partial}{\partial y}, \qquad X_3 = y^2\frac{\partial}{\partial y}. \tag{3.24}$$

According to [17, Example 4.6] there exists exactly one first order differential equation ($y' = 0$) which is invariant under the group of symmetries corresponding to the Lie algebra $\mathbf{g}_3$.

To determine all ordinary differential equations of order $m \geq 2$ which are invariant under the 3-dimensional group of symmetries corresponding to the Lie algebra $\mathbf{g}_3$ we need to compute the 3rd prolonged vector fields $X_i^{(3)}$ of (3.24). Since one has

$$(\phi_1, \phi_2, \phi_3) = (0,0,0), \qquad (\eta_1, \eta_2, \eta_3) = \left(1, y, y^2\right),$$

we obtain

$$\left(\eta_1^{(1)}, \eta_2^{(1)}, \eta_3^{(1)}\right) = \left(0, y', 2yy'\right), \tag{3.25}$$
$$\left(\eta_1^{(2)}, \eta_2^{(2)}, \eta_3^{(2)}\right) = \left(0, y^{(2)}, 2\left(y'\right)^2 + 2yy^{(2)}\right), \tag{3.26}$$
$$\left(\eta_1^{(3)}, \eta_2^{(3)}, \eta_3^{(3)}\right) = \left(0, y^{(3)}, 6y'y^{(2)} + 2yy^{(3)}\right). \tag{3.27}$$

Hence we obtain the system of partial differential equations

$$\begin{aligned} \frac{\partial f}{\partial y} &= 0, \\ y\frac{\partial f}{\partial y} + y'\frac{\partial f}{\partial y'} + y^{(2)}\frac{\partial f}{\partial y^{(2)}} + y^{(3)}\frac{\partial f}{\partial y^{(3)}} &= 0, \\ y^2\frac{\partial f}{\partial y} + 2yy'\frac{\partial f}{\partial y'} + 2\left(\left(y'\right)^2 + yy^{(2)}\right)\frac{\partial f}{\partial y^{(2)}} + 2\left(3y'y^{(2)} + yy^{(3)}\right)\frac{\partial f}{\partial y^{(3)}} &= 0. \end{aligned} \tag{3.28}$$

From the first equation of (3.28) it follows that f does not depend on the variable y. Using this, system (3.28) reduces to

$$\begin{aligned} y'\frac{\partial f}{\partial y'} + y^{(2)}\frac{\partial f}{\partial y^{(2)}} + y^{(3)}\frac{\partial f}{\partial y^{(3)}} &= 0, \\ \left(y'\right)^2\frac{\partial f}{\partial y^{(2)}} + 3y'y^{(2)}\frac{\partial f}{\partial y^{(3)}} &= 0. \end{aligned} \tag{3.29}$$

By integration of the second equation we obtain that its solutions are generated by

$$x, \qquad y', \qquad \alpha = \frac{3}{2}\left(y^{(2)}\right)^2 - y'y^{(3)}. \tag{3.30}$$

Taking the functions in (3.30) as new variables, the vector field $X_2^{(3)} = y'\frac{\partial}{\partial y'} + y^{(2)}\frac{\partial}{\partial y^{(2)}} + y^{(3)}\frac{\partial}{\partial y^{(3)}}$ can be written into the form

$$X_2^{(3)}\left(y'\right)\frac{\partial}{\partial y'} + X_2^{(3)}(\alpha)\frac{\partial}{\partial \alpha} = y'\frac{\partial}{\partial y'} + 2\alpha\frac{\partial}{\partial \alpha}. \tag{3.31}$$

Using integration, the solutions of the partial differential equation

$$y'\frac{\partial f}{\partial y'} + 2\alpha\frac{\partial f}{\partial \alpha} = 0$$

are generated by

$$\varphi_1 = x, \quad \varphi_2 = \frac{\alpha}{\left(y'\right)^2} = \frac{3\left(y^{(2)}\right)^2 - 2y'y^{(3)}}{2\left(y'\right)^2}.$$

Moreover, one has $\varphi_3 = \frac{d\varphi_2}{dx} = \frac{\beta}{(y')^3} = \frac{(y')^2 y^{(4)} + 3\left(y^{(2)}\right)^3 - 4y'y^{(2)}y^{(3)}}{(y')^3}$, and so further. Therefore, any ordinary differential equation of order $m \geq 2$ which is invariant under the action of $\mathbf{g}_3$ actually has order at least 3 and takes the form

$$\Omega\left(x, \varphi_2, \frac{d\varphi_2}{dx}, \frac{d^2\varphi_2}{dx^2}, \ldots\right) = 0,$$

where $\varphi_2 = \frac{3\left(y^{(2)}\right)^2 - 2y'y^{(3)}}{2(y')^2}$, and Ω is an arbitrary function (cf. Theorem 2).

Example 4. The Lie algebra $\mathbf{g}_4 = \mathbf{sl_2}(\mathbb{R})$ is generated by the vector fields

$$X_1 = \frac{\partial}{\partial x}, \quad X_2 = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} \quad, \; X_3 = \left(x^2 - y^2\right)\frac{\partial}{\partial x} + 2xy\frac{\partial}{\partial y}. \tag{3.32}$$

This is the only representation of the Lie algebra $\mathbf{sl_2}(\mathbb{R})$ such that the corresponding group action is primitive on the plane. By [17, Example 4.7] there does not exist any first order differential equation which admits a Lie group of symmetries having the Lie algebra $\mathbf{g}_4$ as its Lie algebra. Because one has

$$(\phi_1, \phi_2, \phi_3) = \left(1, x, x^2 - y^2\right), \quad (\eta_1, \eta_2, \eta_3) = (0, y, 2xy),$$

we obtain

$$\begin{aligned}
\left(\eta_1^{(1)}, \eta_2^{(1)}, \eta_3^{(1)}\right) &= \left(0, 0, 2y\left(1 + (y')^2\right)\right), \\
\left(\eta_1^{(2)}, \eta_2^{(2)}, \eta_3^{(2)}\right) &= \left(0, -y^{(2)}, 2y' + 2(y')^3 + 6yy'y^{(2)} - 2xy^{(2)}\right), \\
\left(\eta_1^{(3)}, \eta_2^{(3)}, \eta_3^{(3)}\right) &= \left(0, -2y^{(3)}, 12(y')^2 y^{(2)} + 6y\left(y^{(2)}\right)^2 + (8yy' - 4x)\, y^{(3)}\right).
\end{aligned}$$

Hence we have the system of partial differential equations

$$\begin{aligned}
\frac{\partial f}{\partial x} &= 0, \\
x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} - y^{(2)}\frac{\partial f}{\partial y^{(2)}} - 2y^{(3)}\frac{\partial f}{\partial y^{(3)}} &= 0, \\
\left(x^2 - y^2\right)\frac{\partial f}{\partial x} + 2xy\frac{\partial f}{\partial y} + 2y\left(1 + (y')^2\right)\frac{\partial f}{\partial y'} & \\
+2\left(y' + (y')^3 + 3yy'y^{(2)} - xy^{(2)}\right)\frac{\partial f}{\partial y^{(2)}} & \\
+2\left(6(y')^2 y^{(2)} + 3y\left(y^{(2)}\right)^2 + (4yy' - 2x)\, y^{(3)}\right)\frac{\partial f}{\partial y^{(3)}} &= 0.
\end{aligned} \tag{3.33}$$

From the first equation of (3.33) it follows that f does not depend on the variable x. Using this, system (3.33) reduces to the following:

$$\begin{aligned}
y\frac{\partial f}{\partial y} - y^{(2)}\frac{\partial f}{\partial y^{(2)}} - 2y^{(3)}\frac{\partial f}{\partial y^{(3)}} &= 0, \\
2y\left(1 + (y')^2\right)\frac{\partial f}{\partial y'} + 2\left(y' + (y')^3 + 3yy'y^{(2)}\right)\frac{\partial f}{\partial y^{(2)}} & \\
+\left(12(y')^2 y^{(2)} + 6y\left(y^{(2)}\right)^2 + 8yy'y^{(3)}\right)\frac{\partial f}{\partial y^{(3)}} &= 0.
\end{aligned} \tag{3.34}$$

By integration of the first equation we obtain that its solutions are generated by

$$y', \quad \alpha = y^{(2)}y, \quad \beta = y^{(3)}y^2. \tag{3.35}$$

Taking the functions in (3.35) as new variables the vector field

$$Y = 2y\left(1+(y')^2\right)\frac{\partial}{\partial y'} + 2\left(y'+(y')^3+3yy'y^{(2)}\right)\frac{\partial}{\partial y^{(2)}} + \left(12(y')^2y^{(2)}+6y\left(y^{(2)}\right)^2+8yy'y^{(3)}\right)\frac{\partial}{\partial y^{(3)}}$$

can be written into the form

$$\widetilde{Y} = \left(1+(y')^2\right)\frac{\partial}{\partial y'} + y'\left(1+(y')^2+3\alpha\right)\frac{\partial}{\partial \alpha} + \left(6(y')^2\alpha+3\alpha^2+4y'\beta\right)\frac{\partial}{\partial \beta}. \tag{3.36}$$

Using integration, the solutions of the partial differential equation

$$\left(1+(y')^2\right)\frac{\partial f}{\partial y'} + y'\left(1+(y')^2+3\alpha\right)\frac{\partial f}{\partial \alpha} + \left(6(y')^2\alpha+3\alpha^2+4y'\beta\right)\frac{\partial f}{\partial \beta} = 0$$

are generated by

$$\begin{aligned}\varphi_1 &= \frac{\alpha+1+(y')^2}{\left(1+(y')^2\right)^{\frac{3}{2}}} = \frac{y^{(2)}y+1+(y')^2}{\left(1+(y')^2\right)^{\frac{3}{2}}},\\ \varphi_2 &= \frac{\beta(y')^2+\beta-3y'\alpha^2}{\left(1+(y')^2\right)^3} = \frac{y^{(3)}y^2\left(1+(y')^2\right)-3y'\left(y^{(2)}\right)^2y^2}{\left(1+(y')^2\right)^3}.\end{aligned} \tag{3.37}$$

Hence any ordinary differential equation of order $m \geq 2$ which is invariant under the action of $\mathbf{g}_4$ takes the form

$$\Omega(\varphi_1, \varphi_2, \dots) = 0,$$

where φ_i, $i = 1, 2$, is given by (3.37), and Ω is an arbitrary function (cf. Theorem 2).

Example 5. The Lie algebra $\mathbf{g}_5 = \mathbb{R}^\mathbf{2} \rtimes \mathbf{sl_2}(\mathbb{R})$ is generated by the vector fields

$$X_1 = \frac{\partial}{\partial x}, \quad X_2 = \frac{\partial}{\partial y}, \quad X_3 = x\frac{\partial}{\partial y}, \quad X_4 = x\frac{\partial}{\partial x} - y\frac{\partial}{\partial y}, \quad X_5 = y\frac{\partial}{\partial x}. \tag{3.38}$$

To determine the ordinary differential equations of order $m \geq 4$ which allow the vector fields X_i, $i = 1, 2, \dots, 5$, given by (3.38) as symmetries, we have to compute the 5th prolonged vector fields $X_i^{(5)}$, $i = 1, 2, \dots, 5$. As one has

$$(\phi_1, \phi_2, \phi_3, \phi_4, \phi_5) = (1, 0, 0, x, y), \tag{3.39}$$

$$(\eta_1, \eta_2, \eta_3, \eta_4, \eta_5) = (0, 1, x, -y, 0), \tag{3.40}$$

we obtain

$$\left(\eta_1^{(1)}, \eta_2^{(1)}, \eta_3^{(1)}, \eta_4^{(1)}, \eta_5^{(1)}\right) = \left(0, 0, 1, -2y', -(y')^2\right), \tag{3.41}$$

$$\left(\eta_1^{(2)}, \eta_2^{(2)}, \eta_3^{(2)}, \eta_4^{(2)}, \eta_5^{(2)}\right) = \left(0, 0, 0, -3y^{(2)}, -3y'y^{(2)}\right), \tag{3.42}$$

$$\left(\eta_1^{(3)}, \eta_2^{(3)}, \eta_3^{(3)}, \eta_4^{(3)}, \eta_5^{(3)}\right) = \left(0, 0, 0, -4y^{(3)}, -4y'y^{(3)} - 3\left(y^{(2)}\right)^2\right), \tag{3.43}$$

$$\left(\eta_1^{(4)}, \eta_2^{(4)}, \eta_3^{(4)}, \eta_4^{(4)}, \eta_5^{(4)}\right) = \left(0, 0, 0, -5y^{(4)}, -5y'y^{(4)} - 10y^{(2)}y^{(3)}\right), \tag{3.44}$$

$$\left(\eta_1^{(5)}, \eta_2^{(5)}, \eta_3^{(5)}, \eta_4^{(5)}, \eta_5^{(5)}\right) = \left(0, 0, 0, -6y^{(5)}, -6y'y^{(5)} - 15y^{(2)}y^{(4)} - 10\left(y^{(3)}\right)^2\right). \tag{3.45}$$

According to Theorem 1, the unique ordinary differential equations of order at most 3 which are invariant under the group of symmetries belonging to the Lie algebra $\mathbb{R}^\mathbf{2} \rtimes \mathbf{sl_2}(\mathbb{R})$ is $y^{(2)} = 0$, because $D = \left|\phi_i,\ \eta_i,\ \eta_i^{(1)},\ \eta_i^{(2)},\ \eta_i^{(3)}\right| = 9\left(y^{(2)}\right)^3$. Moreover, we obtain the system of partial differential equations

$$\begin{aligned}
\frac{\partial f}{\partial x} &= 0, \\
\frac{\partial f}{\partial y} &= 0, \\
x\frac{\partial f}{\partial y} + \frac{\partial f}{\partial y'} &= 0, \\
x\frac{\partial f}{\partial x} - y\frac{\partial f}{\partial y} - 2y'\frac{\partial f}{\partial y'} - \cdots - 6y^{(5)}\frac{\partial f}{\partial y^{(5)}} &= 0, \\
y\frac{\partial f}{\partial x} - \left(y'\right)^2\frac{\partial f}{\partial y'} - 3y'y^{(2)}\frac{\partial f}{\partial y^{(2)}} - \left(4y'y^{(3)} + 3\left(y^{(2)}\right)^2\right)\frac{\partial f}{\partial y^{(3)}}& \\
-5\left(y'y^{(4)} + 2y^{(2)}y^{(3)}\right)\frac{\partial f}{\partial y^{(4)}} - \left(6y'y^{(5)} + 15y^{(2)}y^{(4)} + 10\left(y^{(3)}\right)^2\right)\frac{\partial f}{\partial y^{(5)}} &= 0.
\end{aligned} \tag{3.46}$$

From the first, second and third equations of (3.46) it follows that the function f does not depend on x, y, and y'. The fourth and fifth equations of (3.46) reduce to

$$\begin{aligned}
3y^{(2)}\frac{\partial f}{\partial y^{(2)}} + 4y^{(3)}\frac{\partial f}{\partial y^{(3)}} + 5y^{(4)}\frac{\partial f}{\partial y^{(4)}} + 6y^{(5)}\frac{\partial f}{\partial y^{(5)}} &= 0, \\
3\left(y^{(2)}\right)^2\frac{\partial f}{\partial y^{(3)}} + 10y^{(2)}y^{(3)}\frac{\partial f}{\partial y^{(4)}} + \left(15y^{(2)}y^{(4)} + 10\left(y^{(3)}\right)^2\right)\frac{\partial f}{\partial y^{(5)}} &= 0.
\end{aligned} \tag{3.47}$$

By integration of the second equation of (3.47), we obtain that its solutions are

$$y^{(2)}, \quad \rho_4 = 3y^{(2)}y^{(4)} - 5\left(y^{(3)}\right)^2, \quad \rho_5 = 3\left(y^{(2)}\right)^2 y^{(5)} - 15y^{(2)}y^{(3)}y^{(4)} + \frac{40}{3}\left(y^{(3)}\right)^3. \tag{3.48}$$

Taking the functions in (3.48) as new variables, we can write the vector field corresponding to the first equation of (3.47)

$$B_4 = 3y^{(2)}\frac{\partial f}{\partial y^{(2)}} + 4y^{(3)}\frac{\partial f}{\partial y^{(3)}} + 5y^{(4)}\frac{\partial f}{\partial y^{(4)}} + 6y^{(5)}\frac{\partial f}{\partial y^{(5)}}$$

into the form

$$B_4\left(y^{(2)}\right)\frac{\partial f}{\partial y^{(2)}} + B_4\left(\rho_4\right)\frac{\partial f}{\partial \rho_4} + B_4\left(\rho_5\right)\frac{\partial f}{\partial \rho_5} = 3y^{(2)}\frac{\partial f}{\partial y^{(2)}} + 8\rho_4\frac{\partial f}{\partial \rho_4} + 12\rho_5\frac{\partial f}{\partial \rho_5} = 0. \tag{3.49}$$

The generators of the solutions of (3.49) are

$$\varphi_1 = \rho_4/\left(y^{(2)}\right)^{\frac{8}{3}} = \frac{3y^{(2)}y^{(4)} - 5\left(y^{(3)}\right)^2}{\left(y^{(2)}\right)^{\frac{8}{3}}}, \tag{3.50}$$

$$\varphi_2 = \rho_5/\left(y^{(2)}\right)^4 = \frac{3\left(y^{(2)}\right)^2 y^{(5)} - 15y^{(2)}y^{(3)}y^{(4)} + \frac{40}{3}\left(y^{(3)}\right)^3}{\left(y^{(2)}\right)^4}. \tag{3.51}$$

Moreover, one has $\varphi_3 = \frac{d\varphi_2}{dx}/\frac{d\varphi_1}{dx}$, $\varphi_4 = \frac{d\varphi_3}{dx}/\frac{d\varphi_1}{dx}, \ldots$. According to Theorem 2, any ordinary differential equation of order $m \geq 4$ which is invariant under the group of symmetries belonging to the Lie algebra $\mathbb{R}^{\mathbf{2}} \rtimes \mathbf{sl_2}(\mathbb{R})$ has the form $\Omega\left(\varphi_1, \varphi_2, \varphi_3, \ldots\right) = 0$, where φ_1, φ_2 are given by (3.50), (3.51), and Ω is an arbitrary function.

Example 6. Let $\mathbf{g}_6$ be the 4-dimensional solvable Lie algebra generated by the vector fields

$$X_1 = \frac{\partial}{\partial x}, \quad X_2 = \frac{\partial}{\partial y}, \quad X_3 = y\frac{\partial}{\partial y}, \quad X_4 = x\frac{\partial}{\partial x}. \tag{3.52}$$

To obtain the ordinary differential equations of order at most 2 which allow the group of symmetries corresponding to the Lie algebra $\mathbf{g}_6$, we have to compute the 2nd prolonged vector fields $X_i^{(2)}$, $i = 1, \ldots, 4$. To obtain the invariant differential equations of order $m \geq 3$ we need to compute the 4th prolonged vector fields $X_i^{(4)}$, $i = 1, \ldots, 4$. Since one has

$$(\phi_1, \phi_2, \phi_3, \phi_4) = (1, 0, 0, x), \quad (\eta_1, \eta_2, \eta_3, \eta_4) = (0, 1, y, 0), \tag{3.53}$$

the functions $\eta_i^{(1)}$, $\eta_i^{(2)}$, $\eta_i^{(3)}$, $\eta_i^{(4)}$, $i = 1, 2, 3, 4$, are

$$\left(\eta_1^{(1)}, \eta_2^{(1)}, \eta_3^{(1)}, \eta_4^{(1)}\right) = \left(0, 0, y', -y'\right), \tag{3.54}$$

$$\left(\eta_1^{(2)}, \eta_2^{(2)}, \eta_3^{(2)}, \eta_4^{(2)}\right) = \left(0, 0, y^{(2)}, -2y^{(2)}\right), \tag{3.55}$$

$$\left(\eta_1^{(3)}, \eta_2^{(3)}, \eta_3^{(3)}, \eta_4^{(3)}\right) = \left(0, 0, y^{(3)}, -3y^{(3)}\right), \tag{3.56}$$

$$\left(\eta_1^{(4)}, \eta_2^{(4)}, \eta_3^{(4)}, \eta_4^{(4)}\right) = \left(0, 0, y^{(4)}, -4y^{(4)}\right). \tag{3.57}$$

The determinant $D = \left|\phi_i,\ \eta_i,\ \eta_i^{(1)},\ \eta_i^{(2)}\right|$ in Theorem 1 is $-y'y^{(2)}$. Hence there are two ordinary differential equations of order at most 2 which allow the group of symmetries corresponding to the Lie algebra $\mathbf{g}_6$, namely $y' = 0$ and $y^{(2)} = 0$.

To obtain the invariant differential equations of order $m \geq 3$ we consider the system of partial differential equations

$$\begin{aligned} \frac{\partial f}{\partial x} &= 0, \\ \frac{\partial f}{\partial y} &= 0, \\ y\frac{\partial f}{\partial y} + y'\frac{\partial f}{\partial y'} + \cdots + y^{(4)}\frac{\partial f}{\partial y^{(4)}} &= 0, \\ x\frac{\partial f}{\partial x} - y'\frac{\partial f}{\partial y'} - 2y^{(2)}\frac{\partial f}{\partial y^{(2)}} - 3y^{(3)}\frac{\partial f}{\partial y^{(3)}} - 4y^{(4)}\frac{\partial f}{\partial y^{(4)}} &= 0. \end{aligned} \tag{3.58}$$

The first equation of (3.58) yields that f does not depend on x. The second equation of (3.58) gives that f does not depend on y. This means that $\frac{\partial f}{\partial x} = 0$, $\frac{\partial f}{\partial y} = 0$. Using these, we obtain

$$\begin{aligned} y'\frac{\partial f}{\partial y'} + y^{(2)}\frac{\partial f}{\partial y^{(2)}} + y^{(3)}\frac{\partial f}{\partial y^{(3)}} + y^{(4)}\frac{\partial f}{\partial y^{(4)}} &= 0 \\ y^{(2)}\frac{\partial f}{\partial y^{(2)}} + 2y^{(3)}\frac{\partial f}{\partial y^{(3)}} + 3y^{(4)}\frac{\partial f}{\partial y^{(4)}} &= 0. \end{aligned} \tag{3.59}$$

By integration of the second equation we obtain that its solutions are generated by

$$y', \qquad \gamma = \frac{y^{(3)}}{\left(y^{(2)}\right)^2}, \qquad \delta = \frac{y^{(4)}}{\left(y^{(2)}\right)^3}. \tag{3.60}$$

Taking the functions in (3.60) as new variables the vector field $Y = y'\frac{\partial}{\partial y'} + \cdots + y^{(4)}\frac{\partial}{\partial y^{(4)}}$ can be written into the form

$$Y\left(y'\right)\frac{\partial}{\partial y'} + Y\left(\gamma\right)\frac{\partial}{\partial \gamma} + Y\left(\delta\right)\frac{\partial}{\partial \delta} = y'\frac{\partial}{\partial y'} - \gamma\frac{\partial}{\partial \gamma} - 2\delta\frac{\partial}{\partial \delta}.$$

Using integration, the solutions of the partial differential equation

$$y'\frac{\partial f}{\partial y'} - \gamma\frac{\partial f}{\partial \gamma} - 2\beta\frac{\partial f}{\partial \beta} = 0$$

are generated by

$$\varphi_1 = \gamma y' = \frac{y' y^{(3)}}{\left(y^{(2)}\right)^2}, \quad \varphi_2 = \left(y'\right)^2 \delta = \frac{\left(y'\right)^2 y^{(4)}}{\left(y^{(2)}\right)^3}. \tag{3.61}$$

Furthermore, one has

$$\varphi_3 = \frac{d\varphi_2}{dx} / \frac{d\varphi_1}{dx} = \frac{y^{(5)} \left(y'\right)^2 y^{(2)} + 2y' \left(y^{(2)}\right)^2 y^{(4)} - 3y^{(4)} y^{(3)} \left(y'\right)^2}{y' y^{(4)} \left(y^{(2)}\right)^2 + y^{(3)} \left(y^{(2)}\right)^3 - 2y' y^{(2)} \left(y^{(3)}\right)^2} \tag{3.62}$$

and so on. By Theorem 2 any ordinary differential equations of order $m \geq 3$ which is invariant under the group of symmetries belonging to the Lie algebra $\mathbf{g}_6$ has the form $\Omega\left(\varphi_1, \varphi_2, \varphi_3, \dots\right) = 0$, where φ_1, φ_2 are given by (3.61), and Ω is an arbitrary function.

Chapter 4

Further analysis of cellular pathways: The Lie symmetry group of a second order ordinary differential equation

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Abstract

Motivated by biological examples, we investigate the autonomous second order ordinary differential equation $\ddot{u} = F_0(u) + F_1(u)\dot{u}$, where F_1 is a polynomial in u. We determine that the full Lie group of symmetries of this equation has either 1, 2, 3 or 8 dimensions, and we completely characterize which case occurs depending on F_0 and F_1. Further, when the Lie group has exactly 2 or 3 dimensions, then we provide a basis of the tangential Lie algebra of the symmetry group by infinitesimal generators.

4.1 Introduction

Symmetry analysis is one of the most important tools developed to solve differential equations. Several examples are coming from Physics (see e.g. [40, 7] for comprehensive studies on the topic), and an increasing number of examples are from Biology (see e.g. [37, 15, 38, 39], or [27]). Finding some symmetries for a differential equation can be used to derive an appropriate change of coordinates which then helps to eliminate some of the independent variables or to decrease the order of the system.

We take the FitzHugh–Nagumo model of nerve impulse transmission [27, Chapter 7, p. 177] as a motivation. The "no stimulation" version of this model can be described by the system of first order ordinary differential equations

$$\dot{v} = F(v) - w, \tag{4.1}$$
$$\dot{w} = bv - \gamma w, \tag{4.2}$$

where $F(v) = v(1-v)(v-a)$ is a third order polynomial in v. As every first order system admits an infinite dimensional Lie group, in some cases it might be worthwhile to restrict ourselves to an equivalent second order system, which can only admit a finite dimensional Lie symmetry group. If this Lie group is at least two-dimensional, then pulling it back to the original system could yield two independent symmetries of the original system, and solutions of the original system can be determined by quadratures. This method has been applied successfully in several situations in the past (see e.g. [15, 38, 39] for some recent examples in Biology).

The system (4.1–4.2) is equivalent to the second order ordinary differential equation

$$\ddot{u} = (\gamma F(u) - bu) + \frac{d}{dt}(F(u) - \gamma u), \tag{4.3}$$

which can be obtained by first expressing w from (4.1), substituting it into (4.2) and identifying $v \equiv u$. Now, if (4.3) admits a 2-dimensional Lie symmetry group, then one can express the solutions of the original model by quadratures. Note, that the right-hand side of (4.3) is of the form $F_0(u) + F_1(u)\dot{u}$ for some polynomials $F_0(u) = \gamma F(u) - bu$, $F_1(u) = F'(u) - \gamma$. We take this as our motivation in the following.

In this chapter we consider the second order ordinary differential equation

$$\ddot{u} = F_0(u) + F_1(u)\dot{u}, \tag{4.4}$$

where $F_1(u)$ is a polynomial in u of degree n, and $F_0(u)$ is an arbitrary, infinitely many times differentiable real function of u. Note, that equation (4.4) is autonomous, therefore the tangential Lie algebra $\mathcal{L}$ of the Lie group of all its symmetries always contains the 1-dimensional subalgebra generated by the vector field $\frac{\partial}{\partial t}$. As (4.4) is a second order equation, Lie's method [40, Chapter 2.5] guarantees that determining another generator of $\mathcal{L}$ would then lead to a solution by quadratures of (4.4), and of any first order system equivalent to it.

In Theorem 1 we prove, that (4.4) admits a Lie group of either 1, 2, 3 or 8 dimensions, and we completely characterize the cases where it admits an either 2, 3 or an 8-dimensional Lie group. Further, in the two-dimensional and three-dimensional cases, we provide the generators of the tangential Lie algebra of the Lie group, as well (see Tables 1 and 2 in Section 4.6).

The main result of the chapter is summarized in Theorem 1. Throughout the chapter we consistently keep the convention that coefficients occurring in F_0 are denoted by a_i, and coefficients appearing in F_1 are denoted by b_i, and the degree of F_1 is denoted by n. However, in some of the cases F_0 is not a polynomial, or F_1 can be expressed in a much more compact form by using different constants than its coefficients (see e.g. case (v) of Theorem 1). Therefore in Theorem 1 we decided to consistently use α_i as constants and/or coefficients occurring in F_0, and use β_i as constants and/or coefficients occurring in F_1. Naturally, in the proof we make clear how the a_is and b_is correspond to the α_is and β_is.

Theorem 1. *Let $\mathcal{L}$ be the tangential Lie algebra of the Lie group of all symmetries of the differential equation (4.4), where F_1 is a polynomial, and F_0 is a 4-times continuously differentiable function. Then we have the following.*

I The Lie algebra $\mathcal{L}$ is isomorphic to the 8-dimensional Lie algebra $\mathbf{sl_3}(\mathbb{R})$ if and only if $F_1(u) = \beta_1 u + \beta_0$, $F_0(u) = \alpha_3 u^3 + \alpha_2 u^2 + \alpha_1 u + \alpha_0$, $\alpha_3 = -\frac{1}{9}\beta_1^2$, $\alpha_2 = -\frac{1}{3}\beta_1\beta_0$.

II The Lie algebra $\mathcal{L}$ is isomorphic to the 2-dimensional non-abelian Lie algebra $\mathbf{l_2}(\mathbb{R})$ if and only if we have one of the following cases:

(i) $F_1(u) = \beta_0$, $F_0(u) = \alpha_2 u^2 + \alpha_1 u + \alpha_0$, $\alpha_2 \neq 0$, $\alpha_0 = \frac{\alpha_1^2}{4\alpha_2} - \frac{9\beta_0^4}{625\alpha_2}$;

(ii) $F_1(u) = \beta_0$, $F_0(u) = \alpha_2 e^{\alpha_1 u} + \alpha_0$, $\alpha_2 \neq 0$, $\alpha_1 \neq 0$, $\alpha_0 = \frac{-2\beta_0^2}{\alpha_2}$;

(iii) $F_1(u) = \beta_0$, $F_0(u) = \alpha_3 (u + \alpha_2)^{\alpha_1} + \alpha_0 (u + \alpha_2)$, $\alpha_3 \neq 0$, $\alpha_1 \notin \{-3, 0, 1, 2\}$, $\alpha_0 = \frac{-2\beta_0^2(\alpha_1+1)}{(\alpha_1+3)^2}$;

(iv) $F_1(u) = \beta_1 u + \beta_0$, $F_0(u) = \alpha_3 u^3 + \alpha_2 u^2 + \alpha_1 u + \alpha_0$, $\beta_1 \neq 0$, $\alpha_3 \neq -\frac{1}{9}\beta_1^2$, $\gamma = \frac{\alpha_2\beta_1 - 3\alpha_3\beta_0}{\beta_1^2 + 9\alpha_3}$,

$$\alpha_1 = \gamma^2 + \frac{\beta_0\beta_1 + 3\alpha_2}{\beta_1}\gamma + \frac{\alpha_2\beta_0}{\beta_1},$$

$$\alpha_0 = -\frac{1}{\beta_1}\gamma^3 + \frac{2\beta_0}{3\beta_1}\gamma^2 + \frac{\beta_0^2 + 3\alpha_1}{3\beta_1}\gamma + \frac{\alpha_1\beta_0}{3\beta_1};$$

(v) $F_1(u) = \beta_n(u+\beta_1)^n + \beta_0$, $F_0(u) = \alpha_{2n+1}(u+\beta_1)^{2n+1} + \alpha_{n+1}(u+\beta_1)^{n+1} + \alpha_1(u+\beta_1)$, $n \geq 2$, $\beta_n \neq 0$, $\alpha_{n+1} = \frac{-\beta_0\beta_n}{n+2}$, $\alpha_1 = \frac{-(n+1)\beta_0^2}{(n+2)^2}$.

Here, every α_i, β_i, γ denotes a real number (arbitrary, unless explicitly indicated), while n is a natural number.

III The Lie algebra $\mathcal{L}$ is isomorphic to the 3-dimensional non-abelian Lie algebra $\mathbf{sl_2}(\mathbb{R})$ if and only if we have $F_1(u) = 0$, $F_0(u) = \alpha_1 (u + \alpha_0) + \alpha_{-3} (u + \alpha_0)^{-3}$, $\alpha_{-3} \neq 0$.

IV In any other cases the Lie algebra $\mathcal{L}$ is 1-dimensional.

The symmetry generators in the particular cases are summarized in Tables 1 and 2 of Section 4.6.

The structure of the chapter is the following. In Section 4.2 we derive the symmetry condition for (4.4). In Lemma 2 we show that the infinitesimal generators of a symmetry of (4.4) take the simple form $\xi_u = \eta_{uu} = 0$ (see (4.26)), unless we have case I. Then in Lemma 3 we prove that in case I the Lie algebra $\mathcal{L}$ generated by the infinitesimal generators is isomorphic to the 8-dimensional Lie algebra $\mathbf{sl_3}(\mathbb{R})$, by showing that in these cases (4.4) is equivalent to the equation $\frac{d^2y}{dx^2} = 0$.

The remaining cases are separated into three parts. First, in Section 4.3 we consider the case, where the degree of F_1 is at least 2. We prove item (v), and we obtain that (4.4) admits a 2-dimensional Lie group if and only if F_1 is essentially a shifted power function. Then in Section 4.4 we consider the case where F_1 is linear but not constant, and prove item (iv). Finally, in Section 4.5 we investigate the situation where F_1 is constant, and derive cases (i)–(iii) of Theorem 1. We finish Section 4.5 with a special case, where $F_1 = 0$, F_0 has a term of degree -3, and prove item III. This finishes the complete characterization of symmetries of the equation (4.4). We finish the chapter by listing the second and third generators of $\mathcal{L}$ obtained throughout the calculations in Tables 1 and 2 of Section 4.6.

4.2 The symmetry condition

Consider equation (4.4) on the plane (t, u), where t is the independent and u is the dependent variable. The general form of an infinitesimal generator of a symmetry of (4.4) has the form

$$X = \xi(t,u)\frac{\partial}{\partial t} + \eta(t,u)\frac{\partial}{\partial u}. \tag{4.5}$$

Let D denote the total derivation by t, that is $D\xi = \xi_t + \dot{u}\xi_u$, $D\eta = \eta_t + \dot{u}\eta_u$. We use the convention of writing partial derivatives of a function f into the lower right index of f. Then the first prolongation of X is

$$X^1 = \xi\frac{\partial}{\partial t} + \eta\frac{\partial}{\partial u} + (D\eta - \dot{u}D\xi)\frac{\partial}{\partial \dot{u}}.$$

Further, let

$$S^1 = \frac{\partial}{\partial t} + \dot{u}\frac{\partial}{\partial u} + (F_0 + F_1\dot{u})\frac{\partial}{\partial \dot{u}},$$

be the spray corresponding to the differential equation (4.4). The vector field (4.5) is an infinitesimal symmetry of (4.4) if and only if its first prolongation X^1 satisfies the Lie bracket condition

$$[X^1 - \xi S^1, S^1] = 0 \tag{4.6}$$

on the space $(t, u, \dot{u})$ (cf. [17, Section 3] or [7, Chapter 4, §3]). Substituting X^1 and S^1 into (4.6) we obtain

$$\begin{aligned} 0 &= \left[X^1 - \xi S^1, S^1\right] \\ &= \Big((\eta - \xi\dot{u})(F_0 + F_1\dot{u})_u + (D\eta - \dot{u}D\xi - \xi(F_0 + F_1\dot{u}))(F_0 + F_1\dot{u})_{\dot{u}} - (D\eta - \dot{u}D\xi - \xi(F_0 + F_1\dot{u}))_t \\ &\quad - \dot{u}(D\eta - \dot{u}D\xi - \xi(F_0 + F_1\dot{u}))_u - (F_0 + F_1\dot{u})(D\eta - \dot{u}D\xi - \xi(F_0 + F_1\dot{u}))_{\dot{u}} \Big)\frac{\partial}{\partial \dot{u}}, \end{aligned}$$

therefore

$$\begin{aligned} &F_0'\eta + F_1\eta_t - \eta_{tt} + 2F_0\xi_t - F_0\eta_u \\ &+ \left(F_1'\eta + F_1\xi_t - 2\eta_{tu} + \xi_{tt} + 3F_0\xi_u\right)\cdot\dot{u} \\ &+ (-\eta_{uu} + 2\xi_{tu} + 2F_1\xi_u)\cdot\dot{u}^2 \\ &+ \xi_{uu}\cdot\dot{u}^3 = 0. \end{aligned} \tag{4.7}$$

The left-hand side of (4.7) has to be zero for all $(t, u, \dot{u})$. As ξ, η, F_0, F_1 do not depend on $\dot{u}$, (4.7) is a polynomial in $\dot{u}$. Thus, (4.7) holds if and only if each of its coefficients is zero, that is

$$F_0'\eta + F_1\eta_t - \eta_{tt} + 2F_0\xi_t - F_0\eta_u = 0, \tag{4.8}$$

$$F_1'\eta + F_1\xi_t - 2\eta_{tu} + \xi_{tt} + 3F_0\xi_u = 0, \tag{4.9}$$

$$-\eta_{uu} + 2\xi_{tu} + 2F_1\xi_u = 0, \tag{4.10}$$

$$\xi_{uu} = 0. \tag{4.11}$$

In the following we analyze the system (4.8–4.11).

From (4.11) we have that there exist smooth functions $A(t)$, $B(t)$ such that

$$\xi(t,u) = A(t)u + B(t). \tag{4.12}$$

Then from (4.10) we obtain

$$\eta_{uu}(t,u) = 2A'(t) + 2F_1(u)A(t).$$

Therefore there exist smooth functions $C(t)$, $H(t)$ such that

$$\eta(t,u) = 2A(t)\int\int F_1(u)dudu + A'(t)u^2 + C(t)u + H(t). \tag{4.13}$$

In particular, both ξ and η are polynomial functions in u. In Lemma 2 we prove that $A(t) = 0$ except for case I in Theorem 1.

Lemma 2. *Let $X = \xi(t,u)\frac{\partial}{\partial t} + \eta(t,u)\frac{\partial}{\partial u}$, where $\xi(t,u)$ and $\eta(t,u)$ are given by (4.12) and (4.13), and assume $A(t) \neq 0$. If X is an element of the Lie algebra $\mathcal{L}$ then (4.4) has the form*

$$\ddot{u} = (b_1 u + b_0)\dot{u} + a_3 u^3 + a_2 u^2 + a_1 u + a_0,$$

where a_i, b_i are real constants such that $a_3 = -\frac{1}{9}b_1^2$, $a_2 = -\frac{1}{3}b_1 b_0$.

Proof. First, we show that if $F_1(u)$ is a polynomial of degree $n \geq 2$ in (4.4), and X is an element of $\mathcal{L}$, then $A(t)$ has to be zero. By contradiction, let us suppose $A(t) \neq 0$ in (4.12) and (4.13). Then ξ is a linear polynomial in u and η is a polynomial of degree $n+2$ in u. Substituting (4.12) into (4.9) we have

$$3A(t)F_0 = -F_1'\eta - F_1\xi_t + 2\eta_{tu} - \xi_{tt}, \tag{4.14}$$

Now, the right-hand side of (4.14) is a polynomial in u of degree $(n-1)+(n+2) = 2n+1$, and its leading coefficient comes from the leading coefficient of $-F_1'\eta$. Thus, if $A(t) \neq 0$, then (4.14) can only hold, if F_0 is a polynomial of degree $2n+1$, as well. Let a_{2n+1} denote the leading coefficient of F_0, and c_{n+2} denote the leading coefficient of η.

Now, consider (4.8). The left-hand side of (4.8) is a polynomial in u of degree $3n+2$, and the term for u^{3n+2} comes from the leading terms in $F_0'\eta$ and $F_0\eta_u$. Now, (4.8) can only be satisfied if the leading terms of $F_0'\eta$ and $F_0\eta$ are the same. The leading coefficient of $F_0'\eta$ is $(2n+1)a_{2n+1}c_{n+2}$, the leading coefficient of $F_0\eta_u$ is $(n+2)a_{2n+1}c_{n+2}$. Since $n \geq 2$, $a_{2n+1} \neq 0$, $c_{n+2} \neq 0$ we have $(2n+1)a_{2n+1}c_{n+2} \neq (n+2)a_{2n+1}c_{n+2}$, thus the left-hand side of (4.8) is a polynomial in u of degree $(3n+2)$, which cannot be identically 0 for every t, u, a contradiction.

Thus, the degree n of F_1 is at most 1, or else $A(t) = 0$, and from (4.14) the degree of F_0 is $2n+1 \leq 3$. Thus $F_1(u) = b_1 u + b_0$, $F_0(u) = a_3u^3 + a_2u^2 + a_1u + a_0$ for some real numbers a_i, b_i. Substituting this to (4.13) we have $\eta(t,u) = \frac{1}{3}b_1A(t)u^3 + (b_0A(t) + A'(t))\,u^2 + C(t)u + H(t)$.

Comparing the 3rd and 2nd order terms of (4.14) we obtain

$$\begin{aligned} 3A(t)a_3 &= -b_1 \cdot \frac{1}{3}b_1A(t), \\ 3A(t)a_2 &= -b_1\left(b_0A(t) + A'(t)\right) - b_1A'(t) + 2b_1A'(t). \end{aligned}$$

Hence, if $A(t) \neq 0$, we have $a_3 = -\frac{1}{9}b_1^2$, and $a_2 = -\frac{1}{3}b_1b_0$. □

Lemma 3. *Assume that $F_1(u) = b_1u + b_0$, $F_0(u) = a_3u^3 + a_2u^2 + a_1u + a_0$ such that $a_3 = -\frac{1}{9}b_1^2$, $a_2 = -\frac{1}{3}b_1b_0$. Then the tangential Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4) is isomorphic to the 8-dimensional Lie algebra $\mathbf{sl_3}(\mathbb{R})$.*

Proof. We prove that equation $\frac{d^2y}{dx^2}=0$ can be transformed to (4.4) by a change of variables. According to Lie [31, p. 363–364], after introducing new variables t,u, by the substitution $y=Y(t,u)$ and $x=X(t,u)$ the differential equation $\frac{d^2y}{dx^2}=0$ transforms to

$$\ddot{u}+P\dot{u}^3+(Q+2R)\dot{u}^2+(q+2r)\dot{u}+p=0, \tag{4.15}$$

where

$$P(t,u)=\frac{X_uY_{uu}-Y_uX_{uu}}{X_tY_u-Y_tX_u},\qquad Q(t,u)=\frac{X_tY_{uu}-Y_tX_{uu}}{X_tY_u-Y_tX_u},\qquad R(t,u)=\frac{X_uY_{tu}-Y_uX_{tu}}{X_tY_u-Y_tX_u}, \tag{4.16}$$
$$p(t,u)=\frac{X_tY_{tt}-Y_tX_{tt}}{X_tY_u-Y_tX_u},\qquad q(t,u)=\frac{X_uY_{tt}-Y_uX_{tt}}{X_tY_u-Y_tX_u},\qquad r(t,u)=\frac{X_tY_{tu}-Y_tX_{tu}}{X_tY_u-Y_tX_u}. \tag{4.17}$$

Therefore, the differential equation

$$\ddot{u}=F_1(u)\dot{u}+F_0(u),$$

can be transformed into $\frac{d^2y}{dx^2}=0$ if and only if the system

$$P=0,\qquad Q=-2R,\qquad q+2r=-F_1(u),\qquad p=-F_0(u). \tag{4.18}$$

has a solution. By [31, p. 364] the functions $P(t,u)$, $Q(t,u)$, $R(t,u)$, $p(t,u)$, $q(t,u)$, $r(t,u)$ given by (4.16) and (4.17) satisfy the system of partial differential equations

$$R_u+R^2=0, \tag{4.19}$$
$$-r_u-2R_t+rR=0, \tag{4.20}$$
$$R_t+b_1+2r_u+rR=0, \tag{4.21}$$
$$-F_0'(u)+F_0(u)R-r_t-r^2-rq=0. \tag{4.22}$$

From (4.19) we obtain that $R(t,u)=\frac{1}{u-K(t)}$ with the real smooth function $K(t)$. It follows from (4.20) and (4.21) that $r(t,u)=-\frac{b_1}{3}(u-K(t))+\frac{K'(t)}{u-K(t)}$. Putting $R(t,u)$, $r(t,u)$ and $F_0(u)=a_3u^3+a_2u^2+a_1u+a_0$ into (4.22) we obtain

$$\begin{aligned}&\left(18a_3+2b_1^2\right)u^3+\left(9a_2+3b_1b_0-3b_1^2K(t)-27a_3K(t)\right)u^2-\left(6b_1b_0K(t)+18a_2K(t)\right)u\\&\quad+b_1^2K^3(t)+3b_1b_0K^2(t)-9a_1K(t)-9b_1K(t)K'(t)+9K''(t)-9a_0-9b_0K'(t)=0.\end{aligned} \tag{4.23}$$

Applying $a_3=-\frac{1}{9}b_1^2$, $a_2=-\frac{1}{3}b_1b_0$, we obtain that (4.23) does not depend on u. Further, we have that the function $K(t)$ must satisfy the second order differential equation

$$K''(t)-K'(t)\left(b_1K(t)+b_0\right)-a_3K^3(t)-a_2K^2(t)-a_1K(t)-a_0=0. \tag{4.24}$$

That is, if $K(t)$ is a solution of the original differential equation (4.4), then the system (4.18) has a solution, and the equation $\frac{d^2y}{dx^2}$ can be transformed into (4.4) by a change of variables.

Putting $v(t)=K(t)$, $w(t)=K'(t)$ equation (4.24) is equivalent to the system of first order differential equations

$$v'=w,\qquad w'=(b_1v+b_0)w+a_3v^3+a_2v^2+a_1v+a_0. \tag{4.25}$$

Since the functions w and $(b_1v+b_0)w+a_3v^3+a_2v^2+a_1v+a_0$ are continuous in the variables (t,v,w), for every point (t_0,v_0,w_0) there exists a local solution $K(t)=\varphi(t)$ defined in a suitable neighborhood of t_0 satisfying the initial conditions $\varphi(t_0)=v_0$, $\varphi'(t_0)=w_0$ (cf. [28, p. 66–67]).

With this solution $K(t)=\varphi(t)$, the functions $R(t,u)$ and $r(t,u)$ have the forms $R(t,u)=\frac{1}{u-K(t)}$, $r(t,u)=-\frac{b_1}{3}(u-K(t))+\frac{K'(t)}{u-K(t)}$. Hence by [31, p. 364–365], the differential equation $\frac{d^2y}{dx^2}=0$ can be transformed into (4.4) by a change of variables. □

Lemmas 2 and 3 finish the 'if' part of case I by identifying α_i with a_i and β_i with b_i. The 'only if' part will follow from the other cases. Further, according to Lemma 2, except for case I we have $A(t) = 0$ in (4.12) and in (4.13). Then the generators of the tangential Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4) take the form $X = \xi(t,u)\frac{\partial}{\partial t} + \eta(t,u)\frac{\partial}{\partial u}$ with

$$\xi(t,u) = B(t), \qquad \eta(t,u) = C(t)u + H(t) \tag{4.26}$$

for some smooth real functions $B(t)$, $C(t)$, $H(t)$. We have already made use of equations (4.10–4.11), that is (4.26) is equivalent to satisfying (4.10–4.11). Thus from now on we only need to consider ξ, η of the form (4.26) satisfying (4.8–4.9).

According to the degree n of the polynomial $F_1(u)$ we distinguish three cases. In Section 4.3 we consider the general case $n \geq 2$ (case (v) of Theorem 1). In Section 4.4 we investigate the case $n = 1$ (case (iv) of Theorem 1). Finally, we finish in Section 4.5 by studying $n = 0$ (cases (i)–(iii) of Theorem 1). Note, that in all of these cases we keep the convention of having coefficients b_i in F_1, and (whenever F_0 is a polynomial) coefficients a_i in F_0. These constants are going to be used in the proof, and at the end of each case they will be reformulated using α_is and β_is according to the simpler form in Theorem 1. Further, the integrating constants occurring in ξ and η will be denoted by c_is.

4.3 Degree of F_1 is at least 2

Now, we prove case (v) of Theorem 1. We are searching for ξ, η in the form of (4.26) satisfying (4.8–4.9). Now, (4.9) reduces to

$$0 = (C(t)u + H(t)) \sum_{i=1}^{n} i b_i u^{i-1} + B'(t) \sum_{i=0}^{n} b_i u^i - 2C'(t) + B''(t). \tag{4.27}$$

The right-hand side of (4.27) is a polynomial in u. Collecting the coefficients of this polynomial according to the powers of u we have

$$B''(t) - 2C'(t) + b_0 B'(t) + b_1 H(t) = 0, \quad (0^{\text{th}} \text{ power}), \tag{4.28}$$

$$b_i B'(t) + i b_i C(t) + (i+1) b_{i+1} H(t) = 0, \quad (i^{\text{th}} \text{ power}, \ 1 \leq i \leq n-1), \tag{4.29}$$

$$b_n B'(t) + n b_n C(t) = 0, \quad (n^{\text{th}} \text{ power}). \tag{4.30}$$

For $1 \leq i \leq n$ equations (4.29–4.30) yield a system of homogeneous linear equations with respect to the variables $B'(t)$, $C(t)$ and $H(t)$. The coefficient matrix of this system is

$$M := \begin{pmatrix} b_1 & b_1 & 2b_2 \\ b_2 & 2b_2 & 3b_3 \\ \vdots & \vdots & \vdots \\ b_{n-1} & (n-1)b_{n-1} & nb_n \\ b_n & nb_n & 0 \end{pmatrix}.$$

If the rank of M is 3, then we have $B'(t) = C(t) = H(t) = 0$, $B(t) = c_0 \in \mathbb{R}$. Hence one obtains $\xi(t,u) = c_0 \in \mathbb{R}$, $\eta(t,u) = 0$. Therefore the Lie algebra of the Lie group of all symmetries of (4.4) has dimension 1 and the vector field $Y = \frac{\partial}{\partial t}$ can be chosen as its generator. Otherwise, the rank of M is exactly 2, because the 2×2 determinant

$$\begin{vmatrix} b_{n-1} & nb_n \\ b_n & 0 \end{vmatrix} = -nb_n^2$$

is nonzero. In particular, the first and third column vectors are linearly independent, hence the second column linearly depends on the first and third column vector. Let us denote the column vectors of M by M^1, M^2, M^3. Then there exists λ_1, λ_3 such that

$$M^2 = \lambda_1 M^1 - \lambda_3 M^3.$$

From the last row of M we obtain that $\lambda_1 b_n = nb_n$ and hence $\lambda_1 = n$. The $(n-i)$th row of M, $1 \leq i \leq n-1$, gives that

$$ib_{n-i} = \lambda_3(n-i+1)b_{n-i+1},$$

that is

$$b_{n-i} = \frac{\lambda_3(n-i+1)}{i} b_{n-i+1}.$$

By induction on i we obtain

$$b_{n-i} = \binom{n}{i} \lambda_3^i b_n.$$

Therefore we have

$$F_1(u) = b_0 + \sum_{i=1}^{n} b_n \binom{n}{n-i} \lambda_3^{n-i} u^i = b_n (u+\lambda_3)^n + (b_0 - b_n\lambda_3^n).$$

Thus $F_1(u)$ takes the form

$$F_1(u) = \beta_n(u+\beta_1)^n + \beta_0, \tag{4.31}$$

with $\beta_0 = b_0 - b_n\lambda_3^n$, $\beta_1 = \lambda_3$, $\beta_n = b_n$, where $\beta_n \neq 0$ and $n \geq 2$. Now, (4.9) reduces to

$$\begin{aligned} 0 &= \big(C(t)(u+\beta_1) + H(t) - \beta_1 C(t)\big) n\beta_n (u+\beta_1)^{n-1} + B'(t)\left(\beta_n(u+\beta_1)^n + \beta_0\right) - 2C'(t) + B''(t) \\ &= \beta_n\big(nC(t) + B'(t)\big)(u+\beta_1)^n + n\beta_n\big(H(t) - \beta_1 C(t)\big)(u+\beta_1)^{n-1} + \big(\beta_0 B'(t) - 2C'(t) + B''(t)\big). \end{aligned} \tag{4.32}$$

As (4.32) is a polynomial in $(u+\beta_1)$, all its coefficients must be zero. In particular, we have

$$B'(t) = -nC(t), \tag{4.33}$$

$$H(t) = \beta_1 C(t), \tag{4.34}$$

$$2C'(t) = \beta_0 B'(t) + B''(t). \tag{4.35}$$

In particular, from (4.33–4.34) we have $\xi_t = -nC(t)$, $\eta = C(t)(u+\beta_1)$. Now, substituting (4.33) into (4.35), we obtain

$$C'(t) = \frac{-n\beta_0}{n+2} C(t).$$

Let $\gamma = \frac{-n\beta_0}{n+2}$, then

$$C(t) = c_1 e^{\gamma t}, \tag{4.36}$$

for some constant $c_1 \in \mathbb{R}$.

So far we ensured satisfaction of (4.9). Finally, the functions in (4.33), (4.34) and (4.36) need to satisfy (4.8):

$$\begin{aligned} 0 &= F_0'(u)\left(C(t)u + H(t)\right) + F_0(u)\big(2B'(t) - C(t)\big) + F_1(u)\big(C'(t)u + H'(t)\big) - C''(t)u - H''(t) \\ &= F_0'(u)C(t)(u+\beta_1) - F_0(u)C(t)(2n+1) + C(t)\gamma(u+\beta_1)\left(\beta_n(u+\beta_1)^n + \beta_0\right) - C(t)\gamma^2(u+\beta_1) \\ &= C(t)(u+\beta_1)\left(F_0'(u) - \frac{2n+1}{u+\beta_1}F_0(u) + \gamma\beta_n(u+\beta_1)^n + \gamma\beta_0 - \gamma^2\right). \end{aligned}$$

Either F_0 satisfies the inhomogeneous linear differential equation

$$F_0'(u) - \frac{2n+1}{u+\beta_1}F_0(u) + \gamma\beta_n(u+\beta_1)^n + \gamma\beta_0 - \gamma^2 = 0, \tag{4.37}$$

or else $C(t) = 0$. From the second case $H(t) = 0$, $B'(t) = 0$, $B(t) = c_0 \in \mathbb{R}$ follows. In this case one has $\xi(t,u) = B(t) = c_0 \in \mathbb{R}$ and $\eta(t,u) = 0$, thus (as in the rank-3 case) the tangential Lie algebra of the Lie group of all symmetries of (4.4) is generated by $\frac{\partial}{\partial t}$.

The solution of (4.37) is

$$F_0(u) = \alpha_{2n+1}(u+\beta_1)^{2n+1} + \frac{\gamma\beta_n}{n}(u+\beta_1)^{n+1} + \frac{\gamma\beta_0-\gamma^2}{2n}(u+\beta_1)$$
$$= \alpha_{2n+1}(u+\beta_1)^{2n+1} + \frac{-\beta_0\beta_n}{n+2}(u+\beta_1)^{n+1} + \frac{-(n+1)\beta_0^2}{(n+2)^2}(u+\beta_1),$$

for some $\alpha_{2n+1} \in \mathbb{R}$. If F_0 is of this form, then we obtain

$$\eta(t,u) = c_1 e^{\gamma t}(u+\beta_1),$$
$$\xi(t,u) = c_0 - c_1 n \int e^{\gamma t} dt.$$

In particular, if $\beta_0 = 0$ (i.e. $\gamma = 0$), then the vector fields $Y_1 = \frac{\partial}{\partial t}$, $Y_2 = t\frac{\partial}{\partial t} - \frac{u+\beta_1}{n}\frac{\partial}{\partial u}$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4). If, however, $\beta_0 \neq 0$ (i.e. $\gamma \neq 0$), then the vector fields $Y_1 = \frac{\partial}{\partial t}$, $Y_2 = e^{\gamma t}\left(\frac{\partial}{\partial t} - \gamma\frac{u+\beta_1}{n}\frac{\partial}{\partial u}\right)$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4). This finishes the proof of (v) in Theorem 1.

4.4 Degree of F_1 is 1

In this section, we deal with case (iv) of Theorem 1. We are searching for ξ, η in the form of (4.26) satisfying (4.8–4.9), where $F_1(u) = b_1 u + b_0$, $b_1 \neq 0$. First, consider equation (4.9):

$$\begin{aligned} 0 &= b_1(C(t)u + H(t)) + (b_1 u + b_0)B'(t) - 2C'(t) + B''(t) \\ &= b_1\big(C(t) + B'(t)\big)u + \big(b_1 H(t) + b_0 B'(t) - 2C'(t) + B''(t)\big). \end{aligned} \tag{4.38}$$

Since $b_1 \neq 0$ the coefficient of the term u in (4.38) gives

$$B'(t) = -C(t). \tag{4.39}$$

Hence, from (4.38) we obtain

$$H(t) = \frac{b_0 C(t) + 3C'(t)}{b_1}. \tag{4.40}$$

Applying (4.39) and $F_1(u) = b_1 u + b_0$, equation (4.8) reduces to

$$F_0'(u)(C(t)u + H(t)) - 3F_0(u)C(t) + (b_1 u + b_0)\big(C'(t)u + H'(t)\big) - C''(t)u - H''(t) = 0. \tag{4.41}$$

The third derivation of (4.41) with respect to the variable u is

$$F_0^{(4)}(u)(C(t)u + H(t)) = 0.$$

If $F_0^{(4)} \neq 0$ on some interval, then $C(t)u + H(t) = 0$ on the same interval, and one has $C(t) = H(t) = 0$, hence $B'(t) = 0$. Thus, $B(t) = c_0 \in \mathbb{R}$, the tangential Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4) is 1-dimensional, and is generated by $\frac{\partial}{\partial t}$.

If $F_0^{(4)} \equiv 0$ then the function $F_0(u)$ is an at most 3rd degree polynomial, and has the form

$$F_0(u) = a_3 u^3 + a_2 u^2 + a_1 u + a_0, \tag{4.42}$$

where $a_i \in \mathbb{R}$, $i = 0, 1, 2, 3$. Putting (4.42) into (4.41) and applying (4.40), as well, we obtain

$$u^2\left(\left(\frac{9a_3 + b_1^2}{b_1}\right)C'(t) + \left(\frac{3a_3 b_0 - a_2 b_1}{b_1}\right)C(t)\right)$$

$$+ 2u\left(C''(t) + \left(\frac{b_1b_0+3a_2}{b_1}\right)C'(t) + \left(\frac{a_2b_0-a_1b_1}{b_1}\right)C(t)\right)$$
$$-\frac{3}{b_1}C'''(t) + \frac{2b_0}{b_1}C''(t) + \left(\frac{b_0^2+3a_1}{b_1}\right)C'(t) + \left(\frac{a_1b_0-3a_0b_1}{b_1}\right)C(t) = 0. \quad (4.43)$$

Since (4.43) is a polynomial in u, after multiplying by b_1 we have

$$\left(9a_3+b_1^2\right)C'(t) + (3a_3b_0-a_2b_1)\,C(t) = 0, \quad (4.44)$$
$$b_1C''(t) + (b_1b_0+3a_2)\,C'(t) + (a_2b_0-a_1b_1)\,C(t) = 0, \quad (4.45)$$
$$-3C'''(t) + 2b_0C''(t) + \left(b_0^2+3a_1\right)C'(t) + (a_1b_0-3a_0b_1)\,C(t) = 0. \quad (4.46)$$

If $a_3 = -\frac{1}{9}b_1^2$, and $a_2 = -\frac{1}{3}b_0b_1$, then the tangential Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4) is isomorphic to the 8-dimensional Lie algebra $\mathbf{sl_3}(\mathbb{R})$.

If $a_3 = -\frac{1}{9}b_1^2$, but $a_2 \neq -\frac{1}{3}b_0b_1$, then $9a_3+b_1^2 = 0$, $3a_3b_0-a_2b_1 = -b_1\left(\frac{1}{3}b_1b_0+a_2\right)$. Hence, (4.44) reduces to

$$-b_1\left(\frac{1}{3}b_1b_0+a_2\right)C(t) = 0,$$

which can only be satisfied if $C(t) = 0$, since $a_2 \neq -\frac{1}{3}b_1b_0$, $b_1 \neq 0$. From this $H(t) = 0$, $B'(t) = 0$, $B(t) = c_0 \in \mathbb{R}$ follows. In this case one has $\xi(t,u) = B(t) = c_0 \in \mathbb{R}$ and $\eta(t,u) = 0$, thus the tangential Lie algebra of the Lie group of all symmetries of (4.4) is generated by $\frac{\partial}{\partial t}$.

Hence it remains to investigate the case $a_3 \neq -\frac{1}{9}b_1^2$. Let $\gamma = \frac{a_2b_1-3a_3b_0}{b_1^2+9a_3}$, then the solution of the homogeneous linear differential equation (4.44) is

$$C(t) = c_1e^{\gamma t}, \quad (4.47)$$

for some $c_1 \in \mathbb{R}$. Applying $C^{(i)}(t) = \gamma^iC(t)$, (4.45) and (4.46) translate to

$$C(t)\cdot\big(b_1\gamma^2 + (b_1b_0+3a_2)\,\gamma + (a_2b_0-a_1b_1)\big) = 0, \quad (4.48)$$
$$C(t)\cdot\big(-3\gamma^3 + 2b_0\gamma^2 + \left(b_0^2+3a_1\right)\gamma + (a_1b_0-3a_0b_1)\big) = 0. \quad (4.49)$$

Now, if a_1 and a_0 have values such that either of the big bracketed expressions in (4.48–4.49) attains a nonzero value, then we can conclude $C(t) = 0$. From this $H(t) = 0$, $B'(t) = 0$, $B(t) = c_0 \in \mathbb{R}$ follows. In this case one has $\xi(t,u) = B(t) = c_0 \in \mathbb{R}$ and $\eta(t,u) = 0$, thus the tangential Lie algebra of the Lie group of all symmetries of (4.4) is generated by $\frac{\partial}{\partial t}$.

On the other hand, if both of the big bracketed expressions in (4.48–4.49) are identically zero, then from (4.39–4.40) we obtain

$$H(t) = c_1\frac{b_0+3\gamma}{b_1}e^{\gamma t},$$
$$\eta(t,u) = c_1e^{\gamma t}\left(u+\frac{b_0+3\gamma}{b_1}\right),$$
$$B'(t) = -c_1e^{\gamma t},$$
$$\xi(t,u) = c_0 - c_1\int e^{\gamma t}dt.$$

In particular, if $a_2 = \frac{3a_3b_0}{b_1}$ (i.e. $\gamma = 0$), then the vector fields $Y_1 = \frac{\partial}{\partial t}$, $Y_2 = t\frac{\partial}{\partial t} - \left(u+\frac{b_0}{b_1}\right)\frac{\partial}{\partial u}$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4). If, however, $a_2 \neq \frac{3a_3b_0}{b_1}$ (i.e. $\gamma \neq 0$), then the vector fields $Y_1 = \frac{\partial}{\partial t}$, $Y_2 = e^{\gamma t}\left(\frac{\partial}{\partial t} - \gamma\left(u+\frac{b_0+3\gamma}{b_1}\right)\frac{\partial}{\partial u}\right)$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4).

The big bracketed expression in (4.48) gives a condition on a_1, while the one in (4.49) gives a condition on a_0. Both of these conditions are equivalent to those mentioned in case (iv) in Theorem 1. Putting $\alpha_i = a_i$, $\beta_i = b_i$ finishes the proof of (iv) in Theorem 1.

4.5 Degree of F_1 is 0

The goal of this section is to prove items (i)–(iii) of Theorem 1. We prove case (i) in Section 4.5.1, and cases (ii)–(iii) in Section 4.5.2. Now, we are searching for ξ, η in the form of (4.26) satisfying (4.8–4.9), where $F_1(u) = b_0$. Now, (4.8) takes the form

$$F_0'(u)\left(C(t)u + H(t)\right) + F_0(u)\left(2B'(t) - C(t)\right) + b_0\left(C'(t)u + H'(t)\right) - C''(t)u - H''(t) = 0, \quad (4.50)$$

and (4.9) is of the form

$$b_0 B'(t) - 2C'(t) + B''(t) = 0. \quad (4.51)$$

The first and the second derivative of equation (4.50) with respect to the variable u are respectively

$$F_0''(u)(C(t)u + H(t)) + 2F_0'(u)B'(t) + b_0 C'(t) - C''(t) = 0, \quad (4.52)$$

and

$$F_0'''(u)(C(t)u + H(t)) + F_0''(u)(2B'(t) + C(t)) = 0. \quad (4.53)$$

We distinguish two cases depending on whether F''' is identically 0 or not.

4.5.1 $F_0'''(u) = 0$

We prove case (i) of Theorem 1. If $F_0'''(u) = 0$ then one has $F_0(u) = a_2u^2 + a_1u + a_0$, $a_2, a_1, a_0 \in \mathbb{R}$. If $a_2 = 0$ then equation (4.4) has the form $\ddot{u} = b_0\dot{u} + a_1u + a_0$, and the tangential Lie algebra $\mathcal{L}$ of all symmetries of (4.4) is isomorphic to the 8-dimensional Lie algebra $\mathbf{sl_3}(\mathbb{R})$ by case I of Theorem 1.

Assume $a_2 \neq 0$. Then from (4.53) we obtain that $2a_2(2B'(t) + C(t)) = 0$. Since $a_2 \neq 0$, from (4.53) one has

$$B'(t) = -\frac{1}{2}C(t). \quad (4.54)$$

Substituting (4.54) into (4.51) we conclude that

$$C'(t) = -\frac{b_0}{5}C(t).$$

Let $\gamma = -\frac{b_0}{5}$, then

$$C(t) = c_1 e^{\gamma t} \quad (4.55)$$

for some constant $c_1 \in \mathbb{R}$. Now, substituting (4.54) and $C'(t) = \gamma C(t)$ into (4.52) we obtain

$$H(t) = \frac{a_1 - b_0\gamma + \gamma^2}{2a_2}C(t) = \frac{a_1 + 6\gamma^2}{2a_2}C(t). \quad (4.56)$$

Finally, substituting (4.54), (4.55), and (4.56) into (4.50), we obtain

$$C(t)\left(\frac{a_1 + 6\gamma^2}{2a_2}a_1 - 2a_0 + \frac{a_1 + 6\gamma^2}{2a_2}b_0\gamma - \frac{a_1 + 6\gamma^2}{2a_2}\gamma^2\right) = 0,$$

that is

$$C(t)\left(\frac{a_1^2 - 36\gamma^4}{4a_2} - a_0\right) = 0.$$

Now, if the bracketed expression is not zero, then $C(t) = 0$, yielding $H(t) = B'(t) = 0$. In this case one has $\xi(t,u) = B(t) = c_0 \in \mathbb{R}$ and $\eta(t,u) = 0$, thus the tangential Lie algebra of the Lie group of all symmetries of (4.4) is generated by $\frac{\partial}{\partial t}$.

If, however,

$$a_0 = \frac{a_1^2 - 36\gamma^4}{4a_2} = \frac{a_1^2}{4a_2} - \frac{9b_0^4}{625a_2},$$

then from (4.54–4.56) we obtain

$$\begin{aligned}
H(t) &= c_1 \frac{a_1 + 6\gamma^2}{2a_2} e^{\gamma t},\\
\eta(t,u) &= c_1 e^{\gamma t}\left(u + \frac{a_1 + 6\gamma^2}{2a_2}\right),\\
B'(t) &= -c_1 \frac{1}{2} e^{\gamma t},\\
\xi(t,u) &= c_0 - c_1 \frac{1}{2}\int e^{\gamma t} dt.
\end{aligned}$$

In particular, if $b_0 = 0$ (i.e. $\gamma = 0$), then the vector fields $Y_1 = \frac{\partial}{\partial t}$, $Y_2 = t\frac{\partial}{\partial t} - \left(2u + \frac{a_1}{a_2}\right)\frac{\partial}{\partial u}$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4). If, however, $b_0 \neq 0$ (i.e. $\gamma \neq 0$), then the vector fields $Y_1 = \frac{\partial}{\partial t}$, $Y_2 = e^{\gamma t}\left(\frac{\partial}{\partial t} - \gamma\left(2u + \frac{a_1+6\gamma^2}{a_2}\right)\frac{\partial}{\partial u}\right)$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4). Putting $\alpha_i = a_i$, $\beta_0 = b_0$ finishes the proof of (i) in Theorem 1.

4.5.2 $F_0'''(u) \neq 0$

Assume $F_0'''(u) \neq 0$ on some open subset $U \subseteq \mathbb{R}$. We prove cases (ii)–(iii) of Theorem 1 in this subsection. In particular, we consider case (ii) in Section 4.5.2.1, and deal with case (iii) in Section 4.5.2.2. First we prove that if the Lie symmetry group of (4.4) is at least two-dimensional, then the functions $B'(t)$ and $-\frac{1}{2}C(t)$ must be different. Indeed, if we have $B'(t) = -\frac{1}{2}C(t)$, then from (4.53) we find $-C(t)u = H(t)$. Since the right-hand side of this equation does not depend on u neither can the left-hand side. Hence one has $C(t) = H(t) = 0$, $B(t) = c_0 \in \mathbb{R}$. In this case the tangential Lie algebra $\mathcal{L}$ of all symmetries of (4.4) is only one dimensional and generated by $\frac{\partial}{\partial t}$.

Therefore, let us assume that there exists $B(t)$, $C(t)$ such that for some open subset $T \subseteq \mathbb{R}$ we have $B'(t) \neq -\frac{1}{2}C(t)$ for all $t \in T$. Then (4.53) gives that for all $(t,u) \in T \times U$ we have

$$\frac{F_0''(u)}{F_0'''(u)} = -\frac{C(t)u + H(t)}{2B'(t) + C(t)}. \tag{4.57}$$

As the left-hand side of (4.57) depend only on the variable u so does the right-hand side. Therefore, F_0 satisfies

$$\frac{F_0''(u)}{F_0'''(u)} = s_1 u + s_0 \tag{4.58}$$

for some $s_0, s_1 \in \mathbb{R}$. Note, that $s_1 = s_0 = 0$ is impossible, otherwise $F_0'' = 0$ on U, and thus $F''' = 0$ on U, as well. So from (4.57–4.58) we have

$$H(t) = -2s_0 B'(t) - s_0 C(t), \tag{4.59}$$
$$0 = 2s_1 B'(t) + (s_1 + 1)C(t). \tag{4.60}$$

We distinguish two cases depending on whether $s_1 = 0$ or not.

4.5.2.1 $s_1 = 0, s_0 \neq 0$. We show that item (ii) of Theorem 1 holds. For $s_1 = 0$ we obtain from (4.59–4.60)

$$\begin{aligned}
C(t) &= 0,\\
H(t) &= -2s_0 B'(t).
\end{aligned}$$

Substituting $C(t) = 0$ into (4.51) one obtains

$$B'(t) = c_1 e^{\gamma t},$$

where $\gamma = -b_0$. Thus (4.50) takes the form

$$B'(t)\left(-2s_0F_0'(u) + 2F_0(u) + 2b_0^2s_0 + 2s_0b_0^2\right) = 0. \tag{4.61}$$

Now, either F_0 satisfies the inhomogeneous linear differential equation

$$s_0F_0'(u) - F_0(u) - 2s_0b_0^2 = 0, \tag{4.62}$$

or else from (4.61) we have $B'(t) = 0$, in which case $C(t) = 0$, $H(t) = 0$, $B(t) = c_0 \in \mathbb{R}$ follows. In this case one has $\xi(t,u) = B(t) = c_0 \in \mathbb{R}$ and $\eta(t,u) = 0$, thus the tangential Lie algebra of the Lie group of all symmetries of (4.4) is generated by $\frac{\partial}{\partial t}$.

The solution of (4.62) is

$$\begin{aligned}F_0(u) &= \alpha_2 e^{\frac{1}{s_0}u} - 2b_0^2s_0, \text{ that is}\\ F_0(u) &= \alpha_2 e^{\alpha_1 u} + \alpha_0,\end{aligned}$$

for some $\alpha_2 \in \mathbb{R}$, $\alpha_1 = \frac{1}{s_0}$, $\alpha_0 = -2b_0^2s_0 = \frac{-2b_0}{\alpha_1}$. Note, that $\alpha_2 \neq 0$ (otherwise $F'''(u) = 0$), and $\alpha_1 \neq 0$. Thus we obtain

$$\begin{aligned}\eta(t,u) &= H(t) = c_1\frac{-2}{\alpha_1}e^{\gamma t},\\ \xi(t,u) &= B(t) = c_0 + c_1\int e^{\gamma t}dt.\end{aligned}$$

In particular, if $b_0 = 0$ (i.e. $\gamma = 0$), then the vector fields $Y_1 = \frac{\partial}{\partial t}$, $Y_2 = t\frac{\partial}{\partial t} - \frac{2}{\alpha_1}\frac{\partial}{\partial u}$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4). If, however, $b_0 \neq 0$ (i.e. $\gamma \neq 0$), then the vector fields $Y_1 = \frac{\partial}{\partial t}$, $Y_2 = e^{\gamma t}\left(\frac{\partial}{\partial t} - \frac{2\gamma}{\alpha_1}\frac{\partial}{\partial u}\right)$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4). Putting $\beta_0 = b_0$ finishes the proof of (ii) in Theorem 1.

4.5.2.2 $s_1 \neq 0$. We focus on case (iii) of Theorem 1. From (4.59–4.60) we obtain

$$B'(t) = -\frac{s_1+1}{2s_1}C(t), \tag{4.63}$$

$$H(t) = \frac{s_0}{s_1}C(t). \tag{4.64}$$

Substituting (4.63) first into (4.51), we have

$$0 = -b_0(s_1+1)C(t) - (5s_1+1)C'(t).$$

Now, if $s_1 = -\frac{1}{5}$ (and $b_0 \neq 0$), then we obtain $C(t) = 0$, yielding $H(t) = B'(t) = 0$. In this case one has $\xi(t,u) = B(t) = c_0 \in \mathbb{R}$ and $\eta(t,u) = 0$, thus the tangential Lie algebra of the Lie group of all symmetries of (4.4) is generated by $\frac{\partial}{\partial t}$. We consider the case $s_1 = -\frac{1}{5}$, $b_0 = 0$ in Section 4.5.2.3.

If $s_1 \neq -\frac{1}{5}$, then let $\gamma = -\frac{b_0(s_1+1)}{5s_1+1}$, and we have

$$C(t) = c_1e^{\gamma t}. \tag{4.65}$$

Finally, we substitute (4.63–4.65) into (4.50) to have

$$C(t)\cdot\left(F_0'(u)\left(u + \frac{s_0}{s_1}\right) - \frac{2s_1+1}{s_1}F_0(u) + \left(b_0\gamma - \gamma^2\right)\left(u + \frac{s_0}{s_1}\right)\right) = 0. \tag{4.66}$$

Now, either F_0 satisfies the inhomogeneous linear differential equation

$$F_0'(u)\left(u+\frac{s_0}{s_1}\right)-\frac{2s_1+1}{s_1}F_0(u)+\left(b_0\gamma-\gamma^2\right)\left(u+\frac{s_0}{s_1}\right)=0, \tag{4.67}$$

or (4.66) implies that $C(t)=0$, from which $H(t)=0$, $B'(t)=0$, $B(t)=c_0\in\mathbb{R}$ follows. In this case one has $\xi(t,u)=B(t)=c_0\in\mathbb{R}$ and $\eta(t,u)=0$, thus the tangential Lie algebra of the Lie group of all symmetries of (4.4) is generated by $\frac{\partial}{\partial t}$.

Note, that if $s_1=-1$, then $\gamma=0$, and (4.67) takes the form

$$F_0'(u)\,(u-s_0)-F_0=0.$$

Then the solution of (4.67) is $F_0(u)=\alpha_0\,(u-s_0)$ for some α_0, which contradicts $F_0'''\neq 0$.

Further, if $s_1=-\frac{1}{2}$, then (4.67) takes the form

$$F_0'(u)\,(u-2s_0)+\left(b_0\gamma-\gamma^2\right)(u-2s_0)=0.$$

Then (4.67) gives $F_0'(u)=\gamma^2-b_0\gamma$, which contradicts $F_0'''\neq 0$.

Thus, from now on, we consider only the case $s_1\notin\left\{0,-1,-\frac{1}{2},-\frac{1}{5}\right\}$. Then the solution of (4.67) is

$$\begin{aligned}F_0(u)&=\alpha_3\left(u+\frac{s_0}{s_1}\right)^{\frac{2s_1+1}{s_1}}+\frac{s_1}{s_1+1}\gamma\,(b_0-\gamma)\left(u+\frac{s_0}{s_1}\right), \text{ that is}\\ F_0(u)&=\alpha_3\,(u+\alpha_2)^{\alpha_1}+\alpha_0\,(u+\alpha_2)\,,\end{aligned}$$

for some $\alpha_3\in\mathbb{R}$, $\alpha_2=\frac{s_0}{s_1}$, $\alpha_1=2+\frac{1}{s_1}$, $\alpha_0=\frac{s_1\gamma(b_0-\gamma)}{s_1+1}=\frac{-2b_0^2(\alpha_1+1)}{(\alpha_1+3)^2}$, $\gamma=-\frac{b_0(s_1+1)}{5s_1+1}=\frac{b_0(1-\alpha_1)}{\alpha_1+3}$. Note, that $\alpha_1\notin\{2,1,0,-3\}$, because $s_1\notin\left\{0,-1,-\frac{1}{2},-\frac{1}{5}\right\}$, and $2+\frac{1}{s_1}$ cannot take the value 2 for any s_1. Thus from (4.63–4.65) we obtain

$$\begin{aligned}\eta(t,u)&=C(t)u+H(t)=c_1\,(u+\alpha_2)\,e^{\gamma t},\\ \xi(t,u)&=B(t)=c_0+c_1\frac{1-\alpha_1}{2}\int e^{\gamma t}dt.\end{aligned}$$

In particular, if $b_0=0$ (i.e. $\gamma=0$), then the vector fields $Y_1=\frac{\partial}{\partial t}$, $Y_2=t\frac{\partial}{\partial t}+\frac{2}{1-\alpha_1}\,(u+\alpha_2)\,\frac{\partial}{\partial u}$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4). If, however, $b_0\neq 0$ (i.e. $\gamma\neq 0$), then the vector fields $Y_1=\frac{\partial}{\partial t}$, $Y_2=e^{\gamma t}\left(\frac{\partial}{\partial t}+\frac{2\gamma}{1-\alpha_1}\,(u+\alpha_2)\,\frac{\partial}{\partial u}\right)$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4). Putting $\beta_0=b_0$ finishes the proof of (iii) in Theorem 1.

4.5.2.3 $s_1=-\frac{1}{5}$, $b_0=0$.

Finally, we prove item III of Theorem 1. From (4.59–4.60) we obtain

$$B'(t)=-\frac{s_1+1}{2s_1}C(t)=2C(t), \tag{4.68}$$

$$H(t)=\frac{s_0}{s_1}C(t)=-5s_0C(t). \tag{4.69}$$

Substituting (4.68) first into (4.51), we have

$$0=-b_0(s_1+1)C(t)-(5s_1+1)C'(t),$$

which is an identity, and gives no restriction on $C(t)$. After substituting (4.68–4.69) into (4.50) to have

$$C(t)\left(F_0'(u)\,(u-5s_0)+3F_0(u)\right)=C''(t)\,(u-5s_0)\,. \tag{4.70}$$

Now, $C(t)$ and $C''(t)$ only depend on t, $(F_0'(u)\,(u-5s_0)+3F_0(u))$ and $(u-5s_0)$ only depend on u. Thus, if F_0 does not satisfy the differential equation

$$F_0'(u)\,(u-5s_0)+3F_0(u)=\gamma\,(u-5s_0) \tag{4.71}$$

for some $\gamma\in\mathbb{R}$, then the only solution of (4.70) is $C(t)=0$. From this $H(t)=0$, $B(t)=c_0\in\mathbb{R}$ follows. In this case one has $\xi(t,u)=B(t)=c_0\in\mathbb{R}$ and $\eta(t,u)=0$, thus the tangential Lie algebra of the Lie group of all symmetries of (4.4) is generated by $\frac{\partial}{\partial t}$.

The solution of (4.71) is

$$F_0(u)=a_1\,(u+a_0)+a_{-3}\,(u+a_0)^{-3} \tag{4.72}$$

for some $a_0,a_1,a_{-3}\in\mathbb{R}$ such that $\gamma=4a_1$, $a_0=-5s_0$. Note, that $a_{-3}\neq 0$, otherwise $F'''(u)=0$, with which we have dealt in Section 4.5.1. Now, if F_0 is of the form in (4.72), then (4.70) takes the form

$$\gamma C(t)=C''(t). \tag{4.73}$$

If $\gamma=0$ (i.e. $a_1=0$), then from (4.73), (4.68–4.69) we have

$$\begin{aligned}C(t)&=c_2t+c_1,\\ \eta\,(t,u)&=(c_2t+c_1)\,(u+a_0)\,,\\ \xi\,(t,u)&=c_2t^2+2c_1t+c_0.\end{aligned}$$

Then the vector fields $Y_1=\frac{\partial}{\partial t}$, $Y_2=2t\frac{\partial}{\partial t}+(u+a_0)\,\frac{\partial}{\partial u}$, $Y_3=t^2\frac{\partial}{\partial t}+t\,(u+a_0)\,\frac{\partial}{\partial u}$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4).

If $\gamma>0$ (i.e. $a_1>0$), then from (4.73), (4.68–4.69) we have

$$\begin{aligned}C(t)&=c_2e^{-t\sqrt{\gamma}}+c_1e^{t\sqrt{\gamma}},\\ \eta\,(t,u)&=\left(c_2e^{-t\sqrt{\gamma}}+c_1e^{t\sqrt{\gamma}}\right)(u+a_0)\,,\\ \xi\,(t,u)&=\frac{2\left(c_1e^{t\sqrt{\gamma}}-c_2e^{-t\sqrt{\gamma}}\right)}{\sqrt{\gamma}}+c_0.\end{aligned}$$

Then the vector fields $Y_1=\frac{\partial}{\partial t}$, $Y_2=e^{t\sqrt{\gamma}}\left(2\frac{\partial}{\partial t}+\sqrt{\gamma}\,(u+a_0)\,\frac{\partial}{\partial u}\right)$, $Y_3=e^{-t\sqrt{\gamma}}\left(2\frac{\partial}{\partial t}-\sqrt{\gamma}\,(u+a_0)\,\frac{\partial}{\partial u}\right)$ can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4).

If $\gamma<0$ (i.e. $a_1<0$), then from (4.73), (4.68–4.69) we have

$$\begin{aligned}C(t)&=c_2\cos\left(t\sqrt{-\gamma}\right)+c_1\sin\left(t\sqrt{-\gamma}\right),\\ \eta\,(t,u)&=\left(c_2\cos\left(t\sqrt{-\gamma}\right)+c_1\sin\left(t\sqrt{-\gamma}\right)\right)(u+a_0)\,,\\ \xi\,(t,u)&=\frac{2\,(c_2\sin(t\sqrt{-\gamma})-c_1\cos(t\sqrt{-\gamma}))}{\sqrt{-\gamma}}+c_0.\end{aligned}$$

Then the vector fields $Y_1=\frac{\partial}{\partial t}$, $Y_2=2\cos(t\sqrt{-\gamma})\,\frac{\partial}{\partial t}-\sqrt{-\gamma}\sin(t\sqrt{-\gamma})\,(u+a_0)\,\frac{\partial}{\partial u}$, $Y_3=2\sin(t\sqrt{-\gamma})\,\frac{\partial}{\partial t}+\sqrt{-\gamma}\cos(t\sqrt{-\gamma})\,(u+a_0)\,\frac{\partial}{\partial u}$, can be chosen as the basis elements of the Lie algebra $\mathcal{L}$ of the Lie group of all symmetries of (4.4).

Finally, putting $\alpha_0=a_0$, $\alpha_1=a_1$, $\alpha_{-3}=a_{-3}$ finishes the proof of case III in Theorem 1.

Table 1: The Y_2 generator of $\mathbf{l_2}(\mathbb{R})$ beside $Y_1 = \frac{\partial}{\partial t}$ in cases II

(i) $\beta_0 = 0$	$t\frac{\partial}{\partial t} - \left(2u + \frac{\alpha_1}{\alpha_2}\right)\frac{\partial}{\partial u}$	$[Y_1, Y_2] = Y_1$
(i) $\beta_0 \neq 0$	$e^{\gamma t}\left(\frac{\partial}{\partial t} - \gamma\left(2u + \frac{\alpha_1+6\gamma^2}{\alpha_2}\right)\frac{\partial}{\partial u}\right), \quad \gamma = \frac{-\beta_0}{5}$	$[Y_1, Y_2] = \gamma Y_2$
(ii) $\beta_0 = 0$	$t\frac{\partial}{\partial t} - \frac{2}{\alpha_1}\frac{\partial}{\partial u}$	$[Y_1, Y_2] = Y_1$
(ii) $\beta_0 \neq 0$	$e^{\gamma t}\left(\frac{\partial}{\partial t} - \frac{2\gamma}{\alpha_1}\frac{\partial}{\partial u}\right), \quad \gamma = -\beta_0$	$[Y_1, Y_2] = \gamma Y_2$
(iii) $\beta_0 = 0$	$t\frac{\partial}{\partial t} + \frac{2}{1-\alpha_1}(u + \alpha_2)\frac{\partial}{\partial u}$	$[Y_1, Y_2] = Y_1$
(iii) $\beta_0 \neq 0$	$e^{\gamma t}\left(\frac{\partial}{\partial t} + \frac{2\gamma}{1-\alpha_1}(u + \alpha_2)\frac{\partial}{\partial u}\right), \quad \gamma = \frac{\beta_0(1-\alpha_1)}{\alpha_1+3}$	$[Y_1, Y_2] = \gamma Y_2$
(iv) $\alpha_2 = \frac{3\alpha_3\beta_0}{\beta_1}$	$t\frac{\partial}{\partial t} - \left(u + \frac{\beta_0}{\beta_1}\right)\frac{\partial}{\partial u}$	$[Y_1, Y_2] = Y_1$
(iv) $\alpha_2 \neq \frac{3\alpha_3\beta_0}{\beta_1}$	$e^{\gamma t}\left(\frac{\partial}{\partial t} - \gamma\left(u + \frac{\beta_0+3\gamma}{\beta_1}\right)\frac{\partial}{\partial u}\right), \quad \gamma = \frac{\alpha_2\beta_1-3\alpha_3\beta_0}{\beta_1^2+9\alpha_3}$	$[Y_1, Y_2] = \gamma Y_2$
(v) $\beta_0 = 0$	$t\frac{\partial}{\partial t} - \frac{u+\beta_1}{n}\frac{\partial}{\partial u}$	$[Y_1, Y_2] = Y_1$
(v) $\beta_0 \neq 0$	$e^{\gamma t}\left(\frac{\partial}{\partial t} - \gamma\frac{u+\beta_1}{n}\frac{\partial}{\partial u}\right), \quad \gamma = \frac{-n\beta_0}{n+2}$	$[Y_1, Y_2] = \gamma Y_2$

4.6 Generators of the infinitesimal symmetries

We have summarized the generators of the Lie algebra $\mathcal{L} \simeq \mathbf{l_2}(\mathbb{R})$ in cases II in Table 1. One of the generators is always $Y_1 = \frac{\partial}{\partial t}$, the other generator Y_2 can be read in the second column. Finally, in the third column we listed the Lie bracket $[Y_1, Y_2]$.

We have summarized the generators of the Lie algebra $\mathcal{L} \simeq \mathbf{sl_2}(\mathbb{R})$ in case III in Table 2. One of the generators is always $Y_1 = \frac{\partial}{\partial t}$, the other two generators Y_2 and Y_3 can be read in the second column. Finally, in the third column we listed the Lie brackets $[Y_1, Y_2]$, $[Y_1, Y_3]$, $[Y_2, Y_3]$.

Table 2: The Y_2 and Y_3 generators of $\mathbf{sl_2}(\mathbb{R})$ beside $Y_1 = \frac{\partial}{\partial t}$ in case III

$\alpha_1 = 0$	$Y_2 = 2t\frac{\partial}{\partial t} + (u + \alpha_0)\frac{\partial}{\partial u}$ $Y_3 = t^2\frac{\partial}{\partial t} + t(u + \alpha_0)\frac{\partial}{\partial u}$	$[Y_1, Y_2] = 2Y_1$ $[Y_1, Y_3] = Y_2$ $[Y_2, Y_3] = 2Y_3$
$\alpha_1 > 0$ $\gamma = 4\alpha_1$	$Y_2 = e^{t\sqrt{\gamma}}\left(2\frac{\partial}{\partial t} + \sqrt{\gamma}(u + a_0)\frac{\partial}{\partial u}\right),$ $Y_3 = e^{-t\sqrt{\gamma}}\left(2\frac{\partial}{\partial t} - \sqrt{\gamma}(u + a_0)\frac{\partial}{\partial u}\right)$	$[Y_1, Y_2] = \sqrt{\gamma}Y_2$ $[Y_1, Y_3] = -\sqrt{\gamma}Y_3$ $[Y_2, Y_3] = -8\sqrt{\gamma}Y_1$
$\alpha_1 < 0$ $\gamma = 4\alpha_1$	$Y_2 = 2\cos(t\sqrt{-\gamma})\frac{\partial}{\partial t} - \sqrt{-\gamma}\sin(t\sqrt{-\gamma})(u + a_0)\frac{\partial}{\partial u},$ $Y_3 = 2\sin(t\sqrt{-\gamma})\frac{\partial}{\partial t} + \sqrt{-\gamma}\cos(t\sqrt{-\gamma})(u + a_0)\frac{\partial}{\partial u},$	$[Y_1, Y_2] = -\sqrt{-\gamma}Y_3$ $[Y_1, Y_3] = \sqrt{-\gamma}Y_2$ $[Y_2, Y_3] = 8\sqrt{-\gamma}Y_1$

Chapter 5

Non-Linear Coupling as Colimit

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Coproducts and more generally pushouts and colimits provide in many mathematical realms (i.e., categories) a description of how to combine or 'glue' subsystems together. The coproduct glues together objects with the least possible constraint. In the case of pushouts or colimits, one specifies the 'interface' of the glueing, i.e., constraints on how the components are coupled, using additional morphisms.

In this chapter, we detail these constructions for systems of ordinary differential equations (in the category $\mathcal{ODE}$ introduced in Deliverable 2.1 [36]) in Sections 5.1-5.3, for the category of Interaction Machines in Section 5.4, and for permutation groups and transformation semigroups in Section 5.5, as well as automata with and without outputs in Section 5.6. Nearly all these results (all but the last) appear to be completely new in the scientific literature.

To give intutition the coproduct is generally as similar as possible to disjoint union (as it is for the category of sets and functions), but must yield an object in the category, but may be much harder to describe in other categories. The pushout or colimits can also be understood intuitively from the topological examples: a discrete topological space consisting of two points is mapped to one point by one continuous function, but is also mapped by the (continuous) inclusion function to the end points of a closed interval $[a, b]$ in the real line. The pushout of this diagram is, as a topological space, the circle. The two continuous functions specify that the two points will be collapsed to a single point, but also the two points will be identified with the ends of the interval. Thus, in combining the mentioned spaces according to these constraints, the endpoints will be identified (glued together) in the colimit of this diagram. This corresponds to gluing the two endpoints of a circle together. One can think of the pushout as satisfying the constraint that each image of the singleton space, a single point, will be identified. More generally the maps in the diagrams from which colimits are constructed that what identifications must be made, and the colimit (when it exists), is the least constrained realization of an object in the category that combines all the components in the diagram under the required identifications. Similarly to the circle's construction, higher dimensional manifolds too can be constructed by gluing together simpler pieces. For example, the 2D torus is the colimit of another diagram: A square (just its perimeter) is included in a 'filled in' square (homeomorphic to $[a, b] \times [c, d]$). But the perimeter of the square can be mapped to a figure eight (union of two circles sharing one point) by mapping the top and bottom edge continuously around the top part of the figure eight clockwise and mapping the the left and right edges to the bottom clockwise, so that each corner of the square maps to the shared point. The pushout of this diagram is constrained to 'glue' combine the filled in square and the figure eight according to the constraints that points on the perimeter under the two mappings are identified. The resulting pushout object is homeomorphic to the dimensional surface of a torus ('donut').

Whenever software constraints can be specified by equalities between terms in components to be combined, or by identifications of base components, this gives an interoperability or interface constraints, that a system build from these components must satisfy. The components may be modules, and the way of combining them may be modular in this formalism. But much more general constructions which violated modularity and support or harness interaction are possible to describe in this manner too.

5.1 Preliminaries for the ODEs

An object in the category of **time-dependent first-order ODEs** is defined as a system of equations:

$$\begin{aligned}\frac{dx_1}{dt} &= g(x_1, \cdots, x_n)\\ &\vdots\\ \frac{dx_n}{dt} &= g_n(x_1, \cdots, x_n),\end{aligned} \tag{5.1}$$

which can be summarized as

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{g}(\boldsymbol{x}, t). \tag{5.2}$$

Definition 1. *[36] An α-**morphism of systems of ODEs** $\sigma\colon \Sigma \to \Sigma'$, where Σ has n variables and Σ' has m variables, is a* substitution of variables, *e.g., an algebraic expression in the variables of Σ', or more generally a continuously differentiable function of the variables $(y_1, \ldots, y_m)$ from Σ', for each of the variables x_i of Σ, i.e.,*

$$x_i = \sigma_i(y_1, \ldots, y_m)$$

such that for every equation e in the variables and their derivatives of Σ, with these substitutions $\sigma(e)$ holds in Σ'. Here, $\sigma(e)$ denotes the equation over the variables of Σ' resulting from replacing the variables from Σ in equation e according to the substitution σ.

Remark 1. Two α-morphisms $\sigma, \sigma' : \Sigma \to \Xi$ are equal if and only if for all variables x of Σ, $\sigma(x) = \sigma'(x)$ holds in Ξ (i.e., as a consequence of the equations of of Ξ (without using any equations of Σ)).

Example 1. Let $\Sigma_1\colon \begin{matrix}\dot{w}_1 + \dot{w}_2 = 4w_1 + 2w_2\\ \dot{w}_1 - \dot{w}_2 = 2w_2\end{matrix}$, $\Sigma_2\colon \dot{w}_1 = 2w_1 + 2w_2$ and $\Sigma_3\colon \begin{matrix}\dot{x}_1 = 3x_1 + x_2\\ \dot{x}_2 = x_1 - x_2\end{matrix}$ be ODE systems and f_1, f_2, f_3 and f_4 be defined by the following substitutions,

$f_1\colon \Sigma_1 \to \Sigma_2$ where $\begin{cases} w_1 &= w_1\\ w_2 &= w_2\end{cases}$,

$f_2\colon \Sigma_2 \to \Sigma_1$ where $\begin{cases} w_1 &= w_1\\ w_2 &= w_2\end{cases}$,

$f_3\colon \Sigma_3 \to \Sigma_1$ where $\begin{cases} x_1 &= w_1 + w_2\\ x_2 &= w_1 - w_2\end{cases}$,

$f_4\colon \Sigma_2 \to \Sigma_3$ where $\begin{cases} w_1 &= x_1 + x_2\\ w_2 &= x_1 - x_2\end{cases}$ and

$f_5\colon \Sigma_2 \to \Sigma_3$ where $\begin{cases} w_1 &= \frac{x_1+x_2}{2}\\ w_2 &= \frac{x_1-x_2}{2}\end{cases}$.

Then,

1. The function f_1 is not an α-morphism. If it were, we could compose it with the inclusion of Σ_2 into $\Sigma_2 \cup \{\dot{w}_2 = 1\}$, or with the inclusion of Σ_2 into $\Sigma_2 \cup \{$RHS of eqn 2 of Σ_1 under substitution $f_2 = 1+$ LHS of eqn 2 of Σ_1 under substitution $f_1\}$. This would not allow the equations of Σ_1 to be proved under substitution in the target system. So f_1 cannot be a morphism since the composition would not be one.
2. The function f_2 is an α-morphism. It is an inclusion. In fact, under the (trivial) substitution all equations of Σ_2 hold in Σ_1.

3. The function f_3 is an α-morphism. Indeed, under the substitution f_3 all equations of Σ_3 can be shown to hold in Σ_1. (Note: one is **not** allowed to use the equations of Σ_3 in proving this, only the equations of Σ_1.)
4. The functions f_4 and f_5 are two parallel α-morphisms but they are not equal. That is, one would have to be able to prove under the assumption of just the equations in Σ_3 that $f_4(w_1) = f_5(w_1)$ and $f_4(w_2) = f_5(w_2)$. But that would imply $x_1 + x_2 = 0$ and $x_1 - x_2 = 0$, whence $x_1 = 0 = x_2$, which does not follow from the equations of Σ_3 (since Σ_3 has a non-zero solution). Therefore f_4 and f_5 are not equal as morphisms to Σ_3.

5. However, if the target of f_4 and f_5 is changed as f_6 and f_7 are defined in (5.3), then they are equal. First, since the equation of the source holds after substitution in the target (it reduces to 0=0 under either substitution f_6 or f_7), they are morphisms. Also, these morphisms are equal since $f_6(w_1) = 0 = f_7(w_1)$ and $f_6(w_2) = 0 = f_7(w_2)$ hold in the target.

$$\dot{w}_1 = 2w_1 + 2w_2 \quad \overset{f_6\begin{cases} w_1 & = x_1 + x_2 \\ w_2 & = x_1 - x_2 \end{cases}}{\underset{f_7\begin{cases} w_1 & = \frac{x_1+x_2}{2} \\ w_2 & = \frac{x_1-x_2}{2} \end{cases}}{\rightrightarrows}} \quad \begin{array}{l} \dot{x}_1 = 3x_1 + x_2 \\ \dot{x}_2 = x_1 - x_2 \\ x_1 = x_2 = 0 \end{array} \tag{5.3}$$

Example 2. Let Σ: $\frac{dy}{dx} = \frac{2y}{x}$ and $\hat{\Sigma}$: $\frac{d\hat{y}}{d\hat{x}} = \frac{2\hat{y}}{\hat{x}}$ be two isomorphic ODE systems. Then $\sigma\colon \Sigma \to \hat{\Sigma}$ defined by

$$\begin{cases} x & = \frac{\hat{x}}{\hat{y}} \\ y & = \frac{1}{\hat{y}} \end{cases} \tag{5.4}$$

is an automorphism. Indeed, (5.4) implies that

$$\hat{x} = \frac{x}{y} \text{ and } \hat{y} = \frac{1}{y}. \tag{5.5}$$

Then according to $\hat{\Sigma}$ and (5.5),

$$\frac{d\hat{y}}{d\hat{x}} = \frac{\hat{y}_x dx + \hat{y}_y dy}{\hat{x}_x dx + \hat{x}_y dy} = \frac{0 + \frac{-1}{y^2}dy}{\frac{1}{y}dx + \frac{-x}{y^2}dy} = 2\frac{\frac{1}{y}}{\frac{x}{y}}, \tag{5.6}$$

which implies $\frac{dy}{dx} = \frac{2y}{x}$, that is Σ holds in $\hat{\Sigma}$ and therefore σ is a well-defined α-morphism.

Remark 2. There is an initial object in $\mathcal{ODE}$. It is the empty system of equations with no variables (except time), and no equations. The empty morphism (well, $t = t$) is the unique morphism to any target system.

Remark 3. There is a terminal object too. It is any inconsistent systems of equations, e.g. $1 = 0$ (which is $dt/dt = 0$). In this system any equation is provable. So if $f : \Sigma \to \{0 = 1\}$ is any substitution interpreting the variables of Σ in the those of the target (which include at least t), then the equations of Σ under this substitution hold in the target, since every equation can be proved from $1 = 0$. Thus there is a *unique morphism* since any two substitutions can be proved equal in the target system.

5.2 Coproduct and Pushout of ODE Systems

Proposition 1 (Coproduct of ODE Systems). *Let $\Sigma_X \colon \frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x})$ and $\Sigma_Y \colon \frac{d\boldsymbol{y}}{dt} = \boldsymbol{g}(\boldsymbol{y})$ be two systmes of differential equations. Define the ODE system Σ_Q by the disjoint union of the following systems,*

$$
\begin{aligned}
\frac{d\boldsymbol{x}}{dt} &= \boldsymbol{f}(\boldsymbol{x}) \\
\frac{d\boldsymbol{y}}{dt} &= \boldsymbol{g}(\boldsymbol{y}),
\end{aligned}
\tag{5.7}
$$

and two α-morphisms $i_X \colon \Sigma_X \to \Sigma_Q$ and $i_Y \colon \Sigma_Y \to \Sigma_Q$ by

$$
\begin{aligned}
i_X(\boldsymbol{x}) &= \boldsymbol{x}, \\
i_Y(\boldsymbol{y}) &= \boldsymbol{y}.
\end{aligned}
\tag{5.8}
$$

Then, the ODE system Σ_Q with the morphisms i_X and i_Y is the coproduct of Σ_X and Σ_Y in the category of $\mathcal{ODE}$.

Proof. To prove that Σ_Q is the coproduct of Σ_X and Σ_Y, it should be shown that for any given ODE system Σ_W and α-morphisms $j_X \colon \Sigma_X \to \Sigma_W$ and $j_Y \colon \Sigma_Y \to \Sigma_W$ there is a unique α-morphism $\varphi \colon \Sigma_Q \to \Sigma_W$ for which the following diagram commutes.

$$
\begin{tikzcd}
\Sigma_X \arrow[dr, "i_X"] \arrow[ddr, bend right, "j_X"'] & & \Sigma_Y \arrow[dl, "i_Y"'] \arrow[ddl, bend left, "j_Y"] \\
& \Sigma_Q \arrow[d, dashed, "\varphi"] & \\
& \Sigma_W &
\end{tikzcd}
\tag{5.9}
$$

Suppose Σ_W, j_X and j_Y are given, then define α-morphism φ by

$$
\varphi(q) = \begin{cases} j_X(q), & \text{if } q \text{ is a variable in } \Sigma_X, \\ j_Y(q), & \text{if } q \text{ is a variable in } \Sigma_Y. \end{cases}
\tag{5.10}
$$

Let q be a variable of Σ_Q, then if q is in Σ_X, according to (5.8) and (5.10) $\varphi(i_X(q)) = \varphi(q) = j_X(q)$. Similarly that holds if q is a variable of Σ_Y therefore Diagram 5.9 commutes. Let $\tilde{\varphi}$ be another α-morphism which commutes Diagram 5.9, then $\tilde{\varphi}(q) = \tilde{\varphi}(i_X(q)) = j_X(q) = \varphi(i_X(q)) = \varphi(q)$, if q is a variable of Σ_X and similar result is true for vairables of Σ_Y. Therefore, φ is unique. □

Proposition 2 (Pushout of ODE Systems). *Let $\Sigma_X \colon \frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x})$, $\Sigma_Y \colon \frac{d\boldsymbol{y}}{dt} = \boldsymbol{g}(\boldsymbol{y})$ and $\Sigma_Z \colon \frac{d\boldsymbol{z}}{dt} = \boldsymbol{h}(\boldsymbol{z})$ be three systmes of differential equations, $\sigma_X \colon \Sigma_Y \to \Sigma_X$ and $\sigma_Z \colon \Sigma_Y \to \Sigma_Z$ be two α-morphisms. Define the ODE system Σ_P by the disjoint union of the following systems,*

$$
\begin{aligned}
\frac{d\boldsymbol{x}}{dt} &= \boldsymbol{f}(\boldsymbol{x}) \\
\frac{d\boldsymbol{z}}{dt} &= \boldsymbol{h}(\boldsymbol{z}) \\
\sigma_X(\boldsymbol{x}) &= \sigma_Z(\boldsymbol{z}),
\end{aligned}
\tag{5.11}
$$

and two α-morphisms $i_X : \Sigma_X \to \Sigma_P$ and $i_Z : \Sigma_Z \to \Sigma_P$ by

$$i_X(\boldsymbol{x}) = \boldsymbol{x}, \tag{5.12}$$
$$i_Y(\boldsymbol{y}) = \boldsymbol{y}. \tag{5.13}$$

Then, the ODE system Σ_P with the morphisms i_X and i_Z is the pushout of σ_X and σ_Z in the category of $\mathcal{ODE}$.

Proof. The pushout diagram is commutative, that is $i_X \circ \sigma_X = i_Z \circ \sigma_Z$.

$$\begin{tikzcd}
& \Sigma_Y \arrow[dl, "\sigma_X"'] \arrow[dr, "\sigma_Z"] & \\
\Sigma_X \arrow[dr, "i_X"] \arrow[ddr, bend right, "j_X"'] & & \Sigma_Z \arrow[dl, "i_Z"'] \arrow[ddl, bend left, "j_Z"] \\
& \Sigma_P \arrow[d, dashed, "\varphi"] & \\
& \Sigma_W &
\end{tikzcd} \tag{5.14}$$

Indeed, for every variable y_i in Σ_Y, $(i_X \circ \sigma_X)(y_i)$ is the substitution,

$$y_i = \sigma_{X_i}(x_1, ..., x_n), \tag{5.15}$$

and $(i_Z \circ \sigma_Z)(y_i)$ is the substitution,

$$y_i = \sigma_{Z_i}(z_1, ..., z_k), \tag{5.16}$$

where x_i and z_i s are the variables of Σ_X and Σ_Z, respectively. On the other hand, according to (5.11) $\sigma_{X_i}(x_1, ..., x_n) = \sigma_{Z_i}(z_1, ..., z_k)$ holds in Σ_P, therefore $(i_X \circ \sigma_X)(y_i) = (i_Z \circ \sigma_Z)(y_i)$. Then, the α-moprphism $\varphi \colon \Sigma_P \to \Sigma_W$ is defined as follows which obviously commutes Diagram 5.14. For every variable $p \in \Sigma_P$,

$$\varphi(p) = \begin{cases} j_X(p), & \text{if } p \text{ is a variable in } \Sigma_X, \\ j_Z(p), & \text{if } p \text{ is a variable in } \Sigma_Z. \end{cases} \tag{5.17}$$

Also this φ is unique. In other words, if there is another α-morphism $\tilde{\varphi}$ which commutes Diagram 5.14, then $\tilde{\varphi} \circ i_X = j_X$ and $\tilde{\varphi} \circ i_Z = j_Z$. Since i_X and i_Z are projections on the variables of Σ_X and Σ_Z, respectively, it is obvious that $\tilde{\varphi}(p) = \varphi(p)$ for every variable p in $\Sigma_X \sqcup \Sigma_Z$ which completes the proof. □

Example 3 (Linear and Nonlinear Coupling of Two Spring-Mass Systems as a Pushout). Let us consider two identical systems consisting each of a point mass and spring [11]. The positions of the point masses relative to the equilibirum positions of their respective springs will given by Ψ_a and Ψ_b as functions of time.[18] A term z describes a time-varying coupling between them. But in the system D shown in Figure 5.18 the nature of this coupling is not specificied. In fact the system D specifies the three variables Ψ_a, Ψ_b and z, but gives no constraints at all on them (it has no equations at all, and does not describe the dynamics of either spring-mass system).

[18] This example was developed in collaboration with Paolo Dini.

The system A describes the dynamics of the first spring-mass system with position given by Ψ_a as constrained by the coupling to the second system. But how Ψ_b changes is completely unconstrained in system A. Let k be the spring constant and m the mass of each of the point masses.

On the other side, the system B describes the dynamics of the second spring-mass system with position given by Ψ_b as constrained by a coupling to the first system but with the coupling term having the opposite sign. But how Ψ_a changes is completely unconstrained in system B.

By itself, each of D, A and B is not fully constrained for at least one variable and so has infinitely many solutions given any initial conditions.

The two morphisms (both given by $f = f_A = f_B$ except that the target of f_A is A and that of f_B is B) interpret the coupling as a third spring connecting the point-masses at the ends of the two springs. Here $f_A : D \to B$ and $f_B : D \to B$ both interpret three variables of systems A and B in terms of the variables of D. (Here A, B, and D's variables are regarded as formally distinct.). Since D has no equations, these are trivially morphisms by definition of α-morphism.

$$f : \begin{cases} \Psi_a = \Psi_a \\ \Psi_b = \Psi_b \\ z = \frac{k}{m}(\Psi_b - \Psi_a) \end{cases}$$

$$\begin{tikzcd}
 & \overset{(z, \Psi_a, \Psi_b)}{D} \arrow[dl] \arrow[dr] & \\
A \arrow[r] \arrow[dr, bend right, "T_1"'] & A \sqcup_D B \arrow[d, dashed, "\exists!"] & B \arrow[l] \arrow[dl, bend left, "T_2"] \\
 & C &
\end{tikzcd}$$

$$A: \quad \begin{aligned} \ddot{\Psi}_a &= -\tfrac{k}{m}\Psi_a + z \\ z &= \tfrac{k}{m}(\Psi_b - \Psi_a) \end{aligned} \qquad B: \quad \begin{aligned} \ddot{\Psi}_b &= -\tfrac{k}{m}\Psi_b - z \\ z &= \tfrac{k}{m}(\Psi_b - \Psi_a) \end{aligned}$$

$$A \sqcup_D B: \quad \begin{aligned} \ddot{\Psi}_a &= -\tfrac{k}{m}\Psi_a + z \\ \ddot{\Psi}_b &= -\tfrac{k}{m}\Psi_b - z \\ z &= \tfrac{k}{m}(\Psi_b - \Psi_a) \end{aligned}$$

$$T_2 : \begin{cases} \Psi_a = \frac{\Psi_1 + \Psi_2}{2} \\ \Psi_b = \frac{\Psi_1 - \Psi_2}{2} \\ z = -\frac{k}{m}\Psi_2 \end{cases}$$

$$C: \quad \begin{aligned} \ddot{\Psi}_1 &= -\tfrac{k}{m}\Psi_1 \\ \ddot{\Psi}_2 &= -3\tfrac{k}{m}\Psi_2 \end{aligned} \tag{5.18}$$

The pushout of the diagram $f_A : D \to B$ and $f_B : D \to B$ is the system $A \sqcup_D B$ and describes the dynamics of both spring-mass systems and their coupling together by a third spring along one spatial dimension. Its equations are given on the left-hand side of Figure 5.18. Formally, part of the coproduct is these inclusion morphisms of A and B into this coupled system. The system $A \sqcup_D B$ has the equations of both A and B (and identifies the formally distinct variables with the same name from A and B). It has a unique solution for any initial condition.

The fact that this is a pushout is illustrated by giving another system C with only two variables and morphisms $T_1 : A \to C$ and $T_2 : B \to C$. Note that the equations of A hold in C under the substitution T_1, and similarly the equations of B hold in C when interpreted by the substitution T_2. (In this case, T_1 and T_2 use the same substitution, shown in Figure 5.18)

In fact, C gives the two modes Ψ_1 and Ψ_2 of the two point-masses coupled by a third spring where the point-masses are moving either (1) both always synchronously in the same direction together, or (2) mirror each other's motion, moving always with exactly opposite velocity. The unique morphism interprets Ψ_a, Ψ_b and z in terms of Ψ_1 and Ψ_2 and is in fact an isomorphism of ODE systems. Any solution of this system is a linear superposition of Ψ_1 and Ψ_2.

Another (trivial) linear example would be to replace the equations for z in A and B with $z = 0$, making the two spring-masses independent of each other (in effect, this would be a coproduct).

Moreover, one could replace the original A or B by some other system, such as a pendulum, in which case the pushout would describe the dynamics of a spring-mass system coupled to the pendulum.

Linearly coupled systems of spring-masses or pendulums are well-studied in the literature (see, e.g., [11] for examples and methods of solution), but have not previously been expressed in pushout or colimit form. Expressing coupling of dynamical systems in this manner as a pushout or colimit applies also to nonlinear systems and nonlinear couplings. In principle, we could use a nonlinear coupling z rather than the linear one used here.The resulting pushout would describe this nonlinearly coupled system. In such a case the solutions would no longer be expressible using superposition, and the particular T_1 and T_2 shown would no longer be morphisms to the system C in the Figure. Next we show that the colimit of ODE systems always exists.

5.3 Colimit of ODE Systems

In this section, first we will show how the construction of coequalizer of ODE systems looks like. Then according to [34, p. 113] and Section 5.2 which shows the coproduct of ODE systems exists, we will conclude that the colimit of ODE systems exists.

Lemma 1 (Coequalizer of ODE systems). *Let $f, g\colon \Sigma_1 \rightrightarrows \Sigma_2$ be two α-morphisms where the ODE systems Σ_1 and Σ_2 consist of variables $x_1, \cdots x_n$ and $y_1, \cdots y_m$, respectively. Also, f and g are defined by the substitutions $x_i = f_i(y_1, \cdots, y_m)$ and $x_i = g_i(y_1, \cdots, y_m)$, respectively. Then, the coequalizer of f and g is the inclusion α-morphism $u\colon \Sigma_2 \to \Sigma_2 \cup \Sigma_3$ where Σ_3 is defined by the equations*

$$f_i(y_1, \cdots, y_m) = g_i(y_1, \cdots, y_m), \tag{5.19}$$

for $i = 1, \cdots, n$.

Proof. Let Σ be an ODE system with the $z_1, \cdots, z_k$ variables and $h\colon \Sigma_2 \to \Sigma$ be any α-morphism with the substitution $y_i = h_i(z_1, \cdots, z_k)$ which $h \circ f = h \circ g$. Then, we should show that there is a unique morphism $h'\colon \Sigma_2 \cup \Sigma_3 \to \Sigma$ which commutes Diagram 5.21. The α-morphism h' is defined by the same substitution as h that is

$$y_i = h_i(z_1, \cdots, z_k). \tag{5.20}$$

According to the definition of h' to show that it is well-defined it is sufficient that Σ_3 holds in Σ under h' substitutions. Indeed, $h \circ f = h \circ g$ implies that $f_i\left(h_1(z_1, \cdots, z_k), \cdots, h_m(z_1, \cdots, z_k)\right) = g_i\left(h_1(z_1, \cdots, z_k), \cdots, h_m(z_1, \cdots, z_k)\right)$ holds in Σ. Therefore, under the substitutions of h', that is (5.20), $f_i(y_1, \cdots, y_m) = g_i(y_1, \cdots, y_m)$ holds in Σ. On the other words, according to (5.19) under the substitutions of h', Σ_3 holds in Σ. It is obvious that $h' \circ u = h$. To show the uniqueness suppose there is another α-morphism $h''\colon \Sigma_2 \cup \Sigma_3 \to \Sigma$ which commutes Diagram 5.21 where $x_i = \sigma_i^{h''}(z_1, \cdots, z_k)$. Then, $h'' \circ u = h$ implies that for $i = 1, \cdots, n$, $h''_i(z_1, \cdots, z_k) = h_i(z_1, \cdots, z_k)$ holds in Σ. Therefore, according to (5.20) $h' = h''$.

$$\begin{tikzcd} \Sigma_1 \arrow[r, shift left, "f"] \arrow[r, shift right, "g"'] & \Sigma_2 \arrow[r, "h"] \arrow[d, "u"] & \Sigma \\ & \Sigma_2 \cup \Sigma_3 \arrow[ur, dashed, "\exists h'"'] & \end{tikzcd} \tag{5.21}$$

□

Note: It may well happen that an ODE system has no solution, e.g. $dt/dt = 0$. This is actually a system in which all variables and values are identified (since one can prove $1 = 0$, all quantities are identified). Such a system is a terminal object in $\mathcal{ODE}$. In particular, a coequailzer or coproduct could potentially be (isomorphic) to this object.

Example 4. Let f_4 and f_5 be two parallel α-morphisms as defined in Diagram 5.22. According to Theorem 1 the inclusion morphism u is the coequalizer of f_4 and f_5.

$$\begin{tikzcd}[column sep=huge, row sep=huge] \dot{w}_1 = 2w_1 + 2w_2 \arrow[r, shift left, "f_4\begin{cases} w_1 = x_1+x_2 \\ w_2 = x_1-x_2 \end{cases}"] \arrow[r, shift right, "f_5\begin{cases} w_1 = \frac{x_1+x_2}{2} \\ w_2 = \frac{x_1-x_2}{2} \end{cases}"'] & \begin{array}{l} \dot{x}_1 = 3x_1 + x_2 \\ \dot{x}_2 = x_1 - x_2 \end{array} \arrow[r, "h"] \arrow[d, "u\begin{cases} x_1=x_1 \\ x_2=x_2 \end{cases}"] & \Sigma \\ & \begin{array}{l} \dot{x}_1 = 3x_1 + x_2 \\ \dot{x}_2 = x_1 - x_2 \\ x_1 = x_2 = 0 \end{array} \arrow[ur, dashed, "\exists h'"] & \end{tikzcd} \tag{5.22}$$

For instance, if Σ is the ODE system

$$\begin{aligned} \dot{z}_1 - \dot{z}_2 &= 3z_1 - 3z_2 + z_1^2 - z_2^2 \\ 2z_1\dot{z}_1 - 2z_2\dot{z}_2 &= z_1 - z_2 - z_1^2 + z_2^2 \\ z_1 &= z_2, \end{aligned} \tag{5.23}$$

and $h\colon \begin{array}{l} \dot{x}_1 = 3x_1 + x_2 \\ \dot{x}_2 = x_1 - x_2 \end{array} \longrightarrow \Sigma$ is defined by the substitution $\begin{cases} x_1 = z_1 - z_2 \\ x_2 = z_1^2 - z_2^2 \end{cases}$. Then $h \circ f_4 = h \circ f_5$ and $h'\colon \begin{array}{l} \dot{x}_1 = 3x_1 + x_2 \\ \dot{x}_2 = x_1 - x_2 \\ x_1 = x_2 = 0 \end{array} \longrightarrow \Sigma$ defined by the substitutions $\begin{cases} x_1 = z_1 - z_2 \\ x_2 = z_1^2 - z_2^2 \end{cases}$ commutes Diagram 5.22.

Theorem 1. *The colimit of every finite diagram of ODE Systems exists.*

Proof. According to Proposition 1 and Lemma 1, the coproducts and coequalizers of ODE systems exist and therefore their colimits also exist. □

5.4 Colimits for Interaction Machines as Coalgebras

Here we recall colimit results we proved previously for Interaction Machines formulated as a coalgebraic category. In this section it will be seen that the colimits and limits of $\mathcal{Im}_\bullet$-systems exist. Moreover, the constructions of *coproducts* and *coequalizers* of $\mathcal{I}m_\bullet$-systems are described. Then, according to Mac Lane [34, p. 113] the existence of coproduct and coequalizer implies that every colimit exists. The similar result is true for $\mathcal{I}m^\star$-systems and $\mathcal{D}^\star$-systems. Proofs are in Deliverable D2.2 [29] and omitted here.

By applying [26, Proposition 2.1.5], the coproduct of two interaction machines is obtained as the following,

Theorem 2. *Let $\langle X, \alpha\rangle$ and $\langle Y, \beta\rangle$ be two $\mathcal{I}m_\bullet$-systems. Then, the coproduct of α and β is the $\mathcal{I}m_\bullet$-system $\gamma\colon X \sqcup Y \to \mathcal{I}m_\bullet(X \sqcup Y)$ defined by*

$$\gamma(z) = \begin{cases} (\mathcal{I}m_\bullet(i_X) \circ \alpha)(z), & \text{if } z \in X, \\ (\mathcal{I}m_\bullet(i_Y) \circ \beta)(z), & \text{if } z \in Y, \end{cases} \tag{5.24}$$

where $i_X\colon X \to X \sqcup Y$ and $i_Y\colon Y \to X \sqcup Y$ are inclusion functions.

Proposition 3. *Let $f, g\colon \langle X, \alpha\rangle \rightrightarrows \langle Y, \beta\rangle$ be two $\mathcal{I}m_\bullet$-homomorphisms from $\mathcal{I}m_\bullet$-system α to the $\mathcal{I}m_\bullet$-system β where for each $y \in Y$, $\beta(y) = (\Omega_y, E_y, \Delta_y)$. Then, the coequalizer of f and g is the $\mathcal{I}m_\bullet$-homomorphism $u\colon \langle Y, \beta\rangle \to \langle Y/\sim_{f,g}, \kappa\rangle$ with the following construction: For every $y \in Y$, $u(y) = [y]$ and*
$\kappa\colon Y/\sim_{f,g} \to \mathcal{I}m_\bullet(Y/\sim_{f,g})$ is the $\mathcal{I}m_\bullet$-system defined by $\kappa([y]) = (\Omega_y, E_y, \widetilde{\Delta_y})$ where $[y] \in Y/\sim_{f,g}$ and $\widetilde{\Delta_y}\colon A \to Y$ is defined by $\widetilde{\Delta_y}(a) = [\Delta_y(a)]$ for every $a \in A$.

Proposition 4. *The colimit of every finite $\mathcal{I}m_\bullet$-diagram exists.*

Moreover according to [22], since $\mathcal{I}m_\bullet$ is a bounded functor the product of every two $\mathcal{I}m_\bullet$-systems exists although the construction of the product is not starightforward.

Theorem 3. *The limit of every finite $\mathcal{I}m_\bullet$-diagram exists.*

In particular, the equalizer of two $\mathcal{I}m_\bullet$-systems can be constructed as stated in the following proposition.

Proposition 5. *Let $f, g\colon \langle X, \alpha\rangle \rightrightarrows \langle Y, \beta\rangle$ be two $\mathcal{I}m_\bullet$-homomorphisms from $\mathcal{I}m_\bullet$-system α to the $\mathcal{I}m_\bullet$-system β. Then, the equalizer of f and g is the $\mathcal{I}m_\bullet$-homomorphism $e\colon \langle E, \gamma\rangle \to \langle X, \alpha\rangle$ where $E = \{x \in X\colon \alpha(x) = \beta(x)\}$, $\gamma\colon E \to \mathcal{I}m_\bullet(E)$ is the restriction of α to E and $e(x) = x$ for every $x \in X$.*

5.5 Coproducts for Permutation Groups and Transformation Semigroups

5.5.1 Overview

The structure of coproducts of groups, monoids and semigroups is well-known: they are the so-called "free products" satisfying a universal mapping property and their elements can be written in a canonical form. Surprisingly, the structure of coproducts for faithful representations of groups by permutations, or for monoids and semigroups by transformations appears not to have been described in the literature.[19] Indeed they may fail to exist (in some degenerate cases) for transformation semigroups. Moreover, the most obvious guesses of what the coproduct should be in these categories turn out to be wrong. Here we completely describe the structure of coproducts (including canonical forms for their state sets) in the categories of permutation groups, transformation monoids and transformation semigroups, with or without base point and also for partial transformation semigroups. Also we completely describe the structure of coproducts of automata (whether in the categories of deterministic and complete, or partial automata), i.e. for discrete dynamical systems with inputs, leading to applications for computer science. We also describe the structure of the coproduct of complete deterministic Mealy automata.

5.5.2 Permutation Groups

Objects: A **permutation group** (X, G) is a transformation semigroup in which every element of G is a permutation of elements of X. In addition, for each $g \in G$ there is a $\bar{g} \in G$, such that $g\bar{g} = \bar{g}g = 1_X$. If X is finite, then the second condition is automatically satisfied since some positive power of g will be the identity 1_X on X, i.e., $g^k = 1_X$ for some $k > 1$, in which case $\bar{g} = g^{k-1}$. The transformation $\bar{g}$ is called the **inverse** of g, and is unique.

Morphisms: A **morphism of permutation groups** is a transformation semigroup morphism between permutation groups. Necessarily, it follows that it will map inverses to inverses and also preserve the identity maps.

5.5.3 Transformation Monoids

A transformation semigroup (X, M) is a **transformation monoid** if M contains 1_X, the identity mapping on X. (NB: It is *not* enough to require that M is monoid.)

Morphisms: A morphism $(X, M) \xrightarrow{\varphi} (X', M')$ of transformation monoids is a transformation semigroup morphism which is additionally required to map the identity 1_X on the set X to the identity $1_{X'}$ on X', i.e. $\varphi(1_X) = 1_{X'}$.

Example. The **flip-flop** $(\{a, b\}, FF)$ is a transformation monoid where FF is the monoid consisting of the two constant maps and the identity map on the set $\{a, b\}$.

Remark 4. A transformation semigroup morphism between transformation monoids is not necessarily a transformation monoid morphism. For example, mapping of the flip-flop to itself we can let all states be mapped to state a and all operators map to the constant function taking unique value a.

5.5.4 Transformation Semigroups

Objects: Let X be a set and S be a subsemigroup of X^X, i.e. of all mappings from X to itself. Then (X, S) is a **transformation semigroup**. Notation: If $x \in X$ and $s \in S$ then write $x \cdot s$ for $s(x)$. We

[19] This Section 5.5 is submitted for journal publication and for the reader's convenience first recalls relevant old defintions and also new definitions and concepts from Deliverable D2.1 [36] before introducing the original results on the structure of the coproduct of permutation groups and transformation semigroups. This work was presented at Groups and Topological Groups 2015 in Debrecen, Hungary, the AMS-EMS-SPM International Meeting in Porto, Portugal in June 2015, and the London Mathematical Society – EPSRC Durham Symposium "Permutation Groups and Transformation Semigroups" in July 2015. This section corrects and supersedes the descriptions of the coproduct of transformation semigroups, transformation monoids and permutation groups given in D2.1 [36, pp. 32-33], and the next Section 5.6 also similarly treats the case of complete deterministic automata, and extends the characterization to Mealy automata (automata with outputs) to describe their coproducts too.

have

$$(x \cdot s) \cdot s' = x \cdot ss', \tag{5.25}$$

i.e. ss' denotes the application of s followed by s'. In other words,

$$(ss')(x) = s'(s(x)). \tag{5.26}$$

Here we are using a right action of S on X. Members of X are called **states** and elements of the semigroup S are called **operators**.

Remark 5. Associativity $(st)u = s(tu)$ holds for all elements s, t, u of S since they are functions and function composition is associative. Thus one may unambiguously write stu without parentheses.

Morphisms: A **morphism** $(X, S) \overset{\varphi}{\to} (Y, T)$ **of transformation semigroups** is comprised of two mappings, a function $\varphi^{State} \colon X \to Y$ and a semigroup homomorphism $\varphi^{Operator} \colon S \to T$, compatible with the action. That is,

$$\varphi^{Operator}(s)\varphi^{Operator}(s') = \varphi^{Operator}(ss') \text{ for all } s, s' \in S, \tag{5.27}$$

and, moreover,

$$\varphi^{State}(x) \cdot \varphi^{Operstor}(s) = \varphi^{State}(x \cdot s) \text{ for all } x \in X, s \in S. \tag{5.28}$$

Usually both component maps will simply be denoted by φ.

Notation: Let X, Y be two pointed sets, then $X \vee Y$ denote the disjoint union of X and Y with base-points identified: That is,

$$X \vee Y = (X \setminus \{x_0\}) \sqcup (Y \setminus \{y_0\}) \sqcup \{*\}, \tag{5.29}$$

where x_0, y_0 and $*$ are the base-points of X, Y and $X \vee Y$, respectively. Remark: this set is the pushout of the diagram $X \leftarrow \{*\} \to Y$ of the inclusion maps taking $*$ to the base-points of the sets X and Y.

5.5.5 Coproduct of Groups, Monoids and Semigroups

If S_i are semigroups for all i in some index set I, their **free product** $*_{i \in I} S_i$ is the set of all strings $t_1 t_2 \cdots t_n$, $n \geq 1$ with t_k in some S_i, such that consecutive elements t_k and t_{k+1} do not come from the same S_i (treating the S_i as formally disjoint), which means it is in its unique canonical form. These strings are multiplied by concatenation but if concatenation brings together two elements of the same S_j for some $j \in I$ then these two elements are multiplied in S_j to yield a string of the required form. This is an associative multiplication.

In the case of the categories of monoids or groups, the construction is the same except that one regards the unit elements of all the factors S_i as the *same* element, multiples it by any t_i next to it in the string, then reduces the string by multiplying any neighbouring elements from the same S_i, and iterates if possible. This results again in a canonical form. It is easy to check that this yields a monoid or group, respectively.

Remark 6. Note that when an element $a = u_1 \ldots u_k$ (of length $k \geq 0$) of the group or monoid free product $G * H$ is in the canonical form, then, either $a = 1$ (for $k = 0$), a is a nontrivial member of G or H (for $k = 1$), or the u_i are alternating *non-identity* elements of G or H, $1 \leq i \leq k$. An element $a = u_1 \ldots u_k$ of the semigroup free product $S * T$ in canonical form has length $k \geq 1$, and is either an element of S or T (for $k = 1$) or any alternating sequence members of S and T (when $k > 1$). Moreover, these free products are the coproducts in their respective categories, and every such sequence is the unique canonical form of a member of the coproduct.

Moreover, in each of these categories the free product as such described is the coproduct.

Remark 7. 1. Note that the free product of monoids or groups in the category of semigroups does *not* identify their unit elements, so is different from the free product in the category of monoids.
2. However, the free product of groups in the category of monoids is the same as their free product in the category of groups.
3. The semigroup free product of two or more nontrivial (i.e., non-empty) semigroups is infinite.
4. The semigroup free product of two or more nontriivial semigroups does not have an identity element.
5. The monoid free product of two or more nontrivial monoids (i.e., having more than 1 element each) is infinite. Thus, this free product construction takes one out of the finite realm.

5.5.6 Coproduct of Permutation Groups and Transformation Monoids

Theorem 4. *In the category of permutation groups PermGrp, given permutation groups (X,G) and (Y,H), their coproduct is*

$$((X \sqcup Y) \otimes (G * H), G * H),$$

where $G * H$ is the free product of groups and
$(X \sqcup Y) \otimes (G * H)$ denotes $((X \sqcup Y) \times (G * H))/\equiv$ under the equivalence relation $\equiv$ generated by

$$\begin{aligned} (a, gw) &\sim (a \cdot g, w), \quad \text{if } a \in X, g \in G, \\ (a, hw) &\sim (a \cdot h, w), \quad \text{if } a \in Y, h \in H. \end{aligned} \tag{5.30}$$

We write $a \otimes w$ for the equivalence class of (a,w). Then, $u \in G * H$ acts on $(X \sqcup Y) \otimes (G * H)$ as determined by

$$(a \otimes w) \cdot u = a \otimes wu, \tag{5.31}$$

and $i_X : (X,G) \to ((X \sqcup Y) \otimes (G * H), G * H)$ maps $x \mapsto x \otimes 1$, $g \mapsto g \in G * H$, and $i_Y : (Y,H) \to ((X \sqcup Y) \otimes (G * H), G * H)$ maps $y \mapsto y \otimes 1$, $h \mapsto h \in G * H$. Each element of $(X \sqcup Y) \otimes (G * H)$ can be written as in a canonical form $[a,v]$ where $v = 1$ or a shortest nontrivial member of $G * H$ in canonical form, and a is either

$$\begin{aligned} &a \in X \text{ and } v \neq 1 \text{ does not start with a member of } G, \text{ or,} \\ &a \in Y \text{ and } v \neq 1 \text{ does not start with a member of } H. \end{aligned}$$

Proof. It is clear from (5.30) that each element $a \otimes w$ has a unique canonical form as above since every element of $G*H$ has a unique canonical form as an alternating permutation of elements of G and H. The action is well-defined. Indeed, if $(x, gw) \sim (x \cdot g, w)$, then, $(x, gw) \cdot u = (x, gwu) \sim (x \cdot g, wu) = (x \cdot g, w) \cdot u$ where $u, w \in G * H$. Also, $G * H$ acts faithfully on $(X \sqcup Y) \otimes (G * H)$. First, if one of the groups, say, G is a trivial group then $G * H = H$ and since H acts faithfully on Y therefore it acts faithfully on $(X \sqcup Y) \otimes H$ too. To show the other cases where G and H are not trivial, we exhaustively consider different cases where $u \neq u'$ $(u, u' \in G * H)$ and find a state in $(X \sqcup Y) \otimes (G * H)$ where they disagree:

1. If $u = gw, w = 1$ or starts with $h \in H$ and $u' = g'w'$ where $w' = 1$ or starts with $h' \in H$ and $g \neq g'$, then since (X,G) is faithful, $\exists x \in X, x \cdot g \neq x \cdot g'$. Thus,
$$(x \otimes 1) \cdot u = x \cdot g \otimes w = [x \cdot g, w] \neq [x \cdot g', w'] = (x \otimes 1) \cdot u'.$$
2. If $u = gw$ and $u' = gw'$, where w, w' do not start with an element of G. Then, $u \neq u' \Rightarrow w \neq w'$. Thus,
$$(x \otimes 1) \cdot u = x \cdot g \otimes w = [x \cdot g, w] \neq [x \cdot g, w'] = x \cdot g \otimes w' = (x \otimes 1) \cdot u'.$$

3. If $u = hw$ and $u' = h'w'$, then it is similar to cases 1 and 2.
4. If $u = gw$ and $u' = hw'$ and $\exists x \in X, x \cdot g \neq x$, then

$$(x \otimes 1) \cdot u = x \cdot g \otimes w = [x \cdot g, w] \neq [x, hw'] = x \otimes hw' = (x \otimes 1) \cdot u'.$$

5. If $u = gw$ and $u' = hw'$ and $\forall x \in X, x \cdot g = x$ but $w \neq hw'$, then

$$(x \otimes 1) \cdot u = x \cdot g \otimes w = [x, w] \neq [x, hw'] = (x \otimes 1) \cdot u'.$$

6. If $u = ghw'$ and $u' = hw'$ and $\forall x \in X, x \cdot g = x$, then

$$(y \otimes 1) \cdot u = [y, ghw'] \neq [y \cdot h, w'] = (y \otimes 1) \cdot u'.$$

This establishes faithfulness. The functions $i_{(X,G)}$ and $i_{(Y,H)}$ are injective. Indeed $[x_1, 1] = [x_2, 1]$ implies $x_1 = x_2$ since both are in canonical form. Considering the group component only first, since $G * H$ is the coproduct of groups G and H, i.e. their free product, we take $\varphi^{Operator} \colon G * H \to U$ to be the unique group homomorphism making the group part of the diagram commute.

$$\begin{tikzcd}
(X,G) \arrow[dr, "i_{(X,G)}"] \arrow[ddr, bend right, "j_{(X,G)}"'] & & (Y,H) \arrow[dl, "i_{(Y,H)}"'] \arrow[ddl, bend left, "j_{(Y,H)}"] \\
& ((X \sqcup Y) \otimes (G * H), G * H) \arrow[d, dashed, "\varphi"] & \\
& (Z,U) &
\end{tikzcd} \tag{5.32}$$

The state morphism $\varphi^{State} \colon (X \sqcup Y) \otimes (G * H) \to Z$ is defined by,

$$a \otimes w \mapsto \begin{cases} j_{(X,G)}(a) \cdot \varphi^{Operator}(w), & \text{if } a \in X, \\ j_{(Y,H)}(a) \cdot \varphi^{Operator}(w), & \text{if } a \in Y. \end{cases}$$

It is well-defined since if $(a, w) \sim (a', w')$ then φ^{State} maps them to same $z \in Z$. E.g., $(x, gw) \mapsto j_X(x) \cdot \varphi(gw) = j_X(x) \cdot \varphi(g)\varphi(w) = (j_X(x) \cdot \varphi(g)) \cdot \varphi(w) = (j_X(x) \cdot j_G(g)) \cdot \varphi(w) = j_X(x \cdot g) \cdot \varphi(w)$, which is where (x, gw) maps. The function φ is a morphism, since

$$\begin{aligned} \varphi((a \otimes w) \cdot u) &= \varphi(a \otimes wu) \\ &= j(a) \cdot \varphi(wu) \\ &= j(a) \cdot \varphi(w)\varphi(u) \\ &= (j(a) \cdot \varphi(w)) \cdot \varphi(u) \\ &= \varphi(a \otimes w) \cdot \varphi(u). \end{aligned}$$

The diagram commutes since the group part commutes and $\forall x \in X, x \xmapsto{i_{(X,G)}} [x, 1] \overset{\varphi}{\mapsto} j_{(X,G)}(x)$ and $\forall y \in Y, y \xmapsto{i_{(Y,H)}} [y, 1] \overset{\varphi}{\mapsto} j_{(Y,H)}(y)$. Also, φ is unique. Indeed, if there is another morphism φ_2 that commutes the diagram, then,

$$\begin{aligned} \varphi_2(a \otimes w) &= \varphi_2([a, 1] \cdot w) \\ &= \varphi_2([a, 1]) \cdot \varphi_2(w) \\ &= \varphi_2(i(a)) \cdot \varphi_2(w) \\ &= j(a) \cdot \varphi(w) = \varphi(a \otimes w). \end{aligned}$$

$\square$

Remark 8. The equivalent classes of state set of coproduct can be identified as following:

1. For every $x \in X$,
$$[x, 1] = \{(x'' \cdot g_1, g_2) \colon x'' \cdot g_1 g_2 = x, x'' \in X, g_1, g_2 \in G\}.$$
2. For every $y \in Y$,
$$[y, 1] = \{(y'' \cdot h_1, h_2) \colon y'' \cdot h_1 h_2 = y, y'' \in Y, h_1, h_2 \in H\}.$$
3. For every $x \in X, h \in H$ and $w \in G * H$, not starting with a member of H,
$$[x, hw] = \{(x' \cdot g_1, g_2 hw) \colon x' \cdot g_1 g_2 = x, x' \in X, g_1, g_2 \in G\}.$$
4. For every $y \in Y, g \in G$ and $w \in G * H$, not starting with a member of G,
$$[y, gw] = \{(y' \cdot h_1, h_2 gw) \colon y' \cdot h_1 h_2 = y, y' \in Y, h_1, h_2 \in H\}.$$

Lemma 2. *Let (X, G) and (Y, H) be two pointed permutation groups and $(X \vee Y) \otimes (G * H)$ denote $((X \vee Y) \times (G * H))/\equiv$ under the equivalence relation $\equiv$ generated by*

$$\begin{aligned} (x_0, w) &\sim (y_0, w), && \text{if } x_0, y_0 \text{ are the base-points of } X \text{ and } Y \text{respectively}, \\ (a, gw) &\sim (a \cdot g, w), && \text{if } a \in X, g \in G, \\ (a, hw) &\sim (a \cdot h, w), && \text{if } a \in Y, h \in H, \end{aligned} \tag{5.33}$$

where the base-point of $(X \vee Y) \otimes (G * H)$ is the equivalence class $x_0 \otimes 1 = y_0 \otimes 1$. If, $u \in G * H$ acts on $(X \vee Y) \otimes (G * H)$ as determined by

$$(a \otimes w) \cdot u = a \otimes wu, \tag{5.34}$$

then, each element of $(X \vee Y) \otimes (G * H)$ can be written as in a canonical form $[a, w]$ where $w = 1$ or a shortest nontrivial member of $G * H$ in canonical form, and a is either

$$\begin{aligned} &a \in X \setminus \{x_0\} \text{ and } w \text{ does not start with an element of } G, \text{ or,} \\ &a \in Y \setminus \{y_0\} \text{ and } w \text{ does not start with an element of } H \end{aligned}$$

Proof. To show that each element of $(X \vee Y) \otimes (G * H)$ can be written in the canonical form as stated above we define a reduction system by the following rewriting rules:

$$\begin{aligned} (x, gw) &\mapsto (x \cdot g, w), \\ (y, hw) &\mapsto (y \cdot h, w), \\ (x_0, hw) &\mapsto (y_0, hw), \\ (y_0, gw) &\mapsto (x_0, gw), \end{aligned}$$

where gw and hw are in the $G * H$ canonical form or w can be 1. According to the rewriting rules and the fact that gw and hw are in the canonical form of $G * H$, then each (a, w) can be reduced to a unique normal form (a', w') where non of the rewriting rules can be applied anymore. We denote the normal form of (a, w) by $red(a, w)$. Now we show that if $a \otimes u = a' \otimes u'$ then $red(a, u) = red(a', u')$. Suppose $a \otimes u = a' \otimes u'$, then there exists $a_i \in X \vee Y$ and $u_i \in G * H$ such that $(a, u) \sim (a_1, u_1) \sim \cdots \sim (a_k, u_k) \sim (a', u')$. It is sufficient to show that the equivalence $(a_i, u_i) \sim (a_{i+1}, u_{i+1})$ in one step implies $red(a_i, u_i) = red(a_{i+1}, u_{i+1})$ (we identify $(x_0, 1)$ and $(y_0, 1)$ as $*$). Case one: suppose that $(a_i, u_i) = (x_0, w)$ and $(a_{i+1}, u_{i+1}) = (y_0, w)$. If $w = 1$ then $red(x_0, 1) = red(y_0, 1) = *$. Otherwise, if $w = hw'$ then $(x_0, w) = (x_0, hw') \mapsto (y_0, hw') = (y_0, w)$ i.e. $red(x_0, w) = red(y_0, w)$. Similarly, if $w = gw'$, then $red(y_0, w) = red(y_0, gw') = red(x_0, gw') = red(x_0, w)$. Case two: suppose $(x, gw) \sim (x \cdot g, w)$ where

$x \in X$. If $w = 1$, then $(x, gw) = (x, g) \mapsto (x{\cdot}g, 1)$ i.e., $red(x, g) = red(x{\cdot}g, 1)$. If $w \neq 1$ and the canonical form of it in $G * H$ denoted by $Can(w) = hw'$, then $(x, gw) = (x, ghw') \mapsto (x \cdot g, hw') = (x \cdot g, w)$, i.e $red(x, gw) = red(x \cdot g, w)$. Otherwise, if $Can(w) = g'w''$, then $(x, gw) = (x, gg'w'') \mapsto (x \cdot gg', w'')$. On the other hand, $(x \cdot g, w) = (x \cdot g, g'w'') \mapsto (x \cdot gg', w'')$ therefore, $red(x \cdot g, w) = (x, gw)$. Case three: suppose $(y, hw) \sim (y \cdot h, w)$ where $y \in Y$, which is similar to case two. Therefore, since neighbouring members $(a_i, u_i) \sim (a_{i+1}, u_{i+1})$ in an equivalence chain reduced to the same canonical form, so it follows that equivalent (a, u)'s have the same canonical form. (And conversely same canonical form implies equivalence.) □

Theorem 5. *In the categories of pointed permutation groups $PermGrp_*$, given pointed permutation groups (X, G) and (Y, H), their coproduct is*

$$((X \vee Y) \otimes (G * H), G * H),$$

where $G * H$ is the free product of groups and $(X \vee Y) \otimes (G * H)$ is defined as in Lemma 2, $i_X : (X, G) \to ((X \vee Y) \otimes (G * H), G * H)$ maps $x \mapsto x \otimes 1$, $g \mapsto g \in G * H$, and $i_Y : (Y, H) \to ((X \vee Y) \otimes (G * H), G * H)$ maps $y \mapsto y \otimes 1$, $h \mapsto h \in G * H$. Then, $u \in G * H$ acts on $(X \vee Y) \otimes (G * H)$ as determined by

$$(a \otimes w) \cdot u = a \otimes wu. \tag{5.35}$$

Each element of $(X \vee Y) \otimes (G * H)$ can be written in a unique canonical form as stated in Lemma 2.

Proof. The action is well-defined. Indeed,

$$\begin{aligned}
(x_0, w) \sim (y_0, w) &\Rightarrow (x_0, w) \cdot u = (x_0, wu) \sim (y_0, wu) = (y_0, w) \cdot u,\\
(x, gw) \sim (x \cdot g, w) &\Rightarrow (x, gw) \cdot u = (x, gwu) \sim (x \cdot g, wu) = (x \cdot g, w) \cdot u,\\
(y, hw) \sim (y \cdot h, w) &\Rightarrow (y, hw) \cdot u = (y, hwu) \sim (y \cdot h, wu) = (y \cdot h, w) \cdot u.
\end{aligned}$$

Also, $G * H$ acts faithfully on $(X \vee Y) \otimes (G * H)$. We may assume that $|X|, |Y| > 1$, otherwise, if $|X|$ or $|Y| = 1$, say, $|X| = 1$ then, G must be the trivial group and therefore $G * H \cong H$ and it acts faithfully on $(\{x_0\} \vee Y) \otimes H$, which is in natural one-to-one correspondence to Y, i.e. in this case the coproduct is isomorphic to (Y, H). To show the other cases where $|X|, |Y| > 1$ we consider different cases where $u \neq u'$ $(u, u' \in G * H)$ and find a state in $(X \vee Y) \otimes (G * H)$ where they disagree:

1. If $u = gw, w = 1$ or starts with $h \in H$ and $u' = g'w'$ where $w' = 1$ or starts with $h' \in H$, then take any $x \neq x_0 \in X$ and $h_1 \in H$. Thus,

$$(x \otimes h_1) \cdot u = [x, h_1 gw] \neq [x, h_1 g'w'] = (x \otimes h_1) \cdot u'.$$

2. If $u = hw$ and $u' = h'w'$, then it is similar to case 1.
3. If $u = gw, w = 1$ or starts with $h \in H$ and $u' = h'w', w' = 1$ or starts with $g' \in G$ and $\exists x \neq x_0 \in X, x \cdot g \neq x$, then

$$(x \otimes 1) \cdot u = x \cdot g \otimes w = [x \cdot g, w] \neq [x, h'w'] = x \otimes h'w' = (x \otimes 1) \cdot u'.$$

4. If $u = gw, w = 1$ or starts with $h \in H$ and $u' = h'w', w' = 1$ or starts with $g' \in G$ and $\forall x \neq x_0 \in X, x \cdot g = x$ but $w \neq h'w'$, then

$$(x \otimes 1) \cdot u = x \cdot g \otimes w = [x, w] \neq [x, h'w'] = (x \otimes 1) \cdot u'.$$

5. If $u = ghw'$ and $u' = hw'$ where $w' = 1$ or starts with $g' \in G$ and $\forall x \neq x_0 \in X, x \cdot g = x$, then

$$(y \otimes 1) \cdot u = [y, ghw'] \neq [y \cdot h, w'] = (y \otimes 1) \cdot u'.$$

This establishes faithfulness. Similar to the proof of Theorem 4, considering the group component only first,we take $\varphi^{Operator}\colon G * H \to U$ to be the unique group homomorphism making the group part of Diagram 5.32 commute. Then, the state morphism $\varphi^{State}\colon (X \vee Y) \otimes (G * H) \to Z$ is defined by,

$$[a, w] \mapsto \begin{cases} z_0 \cdot \varphi^{Operator}(w) & \text{if } a \in \{x_0, y_0\}, \\ j_{(X,G)}(a) \cdot \varphi^{Operator}(w), & \text{if } a \in X, \\ j_{(Y,H)}(a) \cdot \varphi^{Operator}(w), & \text{if } a \in Y. \end{cases}$$

Similar to the proof of Theorem 4, φ is a well-defined morphism. Also, $\varphi(i(a)) = \varphi(a, 1) = j(a) \cdot \varphi^{Operator}(1) = j(a) \cdot 1 = j(a)$ where $a \notin \{x_0, y_0\}$. If $a = x_0$ or y_0, then $\varphi(i(a)) = \varphi([a, 1]) = z_0 \cdot \varphi^{Operator}(1) = z_0 = j(a)$. It is streightforward to check that φ is unique. □

Theorem 6. *Let (X, M) and (Y, N) be in the category of transformations monoids TM. Then their coproduct is $((X \times (M * N)) \sqcup (Y \times (M * N)))/\equiv, M * N)$, where $M * N$ is the free product of monoids and $\equiv$ is the transitive closure of $\sim$ defined by,*

$$\begin{aligned} (a, sw) &\sim (a \cdot s, w), \quad \textit{if } a \in X, s \in M, \\ (a, tw) &\sim (a \cdot t, w), \quad \textit{if } a \in Y, t \in N. \end{aligned} \tag{5.36}$$

Theorem 7. *In the categories of pointed transformations monoids TM_* let (X, M) and (Y, N) be pointed transformation monoids not necessarily faithful. Then their coproduct is $((X \times (M * N)) \sqcup (Y \times (M * N)))/\equiv, M * N)$, where $M * N$ is the free product of monoids and $\equiv$ is the transitive closure of $\sim$ defined by,*

$$\begin{aligned} (x_0, w) &\sim (y_0, w), && \textit{if } x_0, y_0 \textit{ are the base-points of } X \textit{ and } Y, \textit{respectively}, \\ (a, sw) &\sim (a \cdot s, w), && \textit{if } a \in X, s \in S, \\ (a, tw) &\sim (a \cdot t, w), && \textit{if } a \in Y, t \in T. \end{aligned} \tag{5.37}$$

5.5.7 Coproduct of Transformation Semigroups

Notation: we denote the empty string by λ. Also, $(S * T)^\lambda$ means $(S * T) \sqcup \{\lambda\}$ where λ is not an element of $S * T$. We shall write $\lambda w = w = w\lambda$. (In fact this makes $S * T$ into a monoid with a new identity element λ.)

Theorem 8 (Coproduct Transformation Semigroups). *Let (X, S) and (Y, T) be in TS except the case both S and T are nonempy semigroups acting on empty sets $X = Y = \emptyset$. Then, the coproduct is given by the natural inclusions (X, S) and (Y, T) in $(Q, S * T)$ where the coproduct state Q is given by,*

$$((X \sqcup Y) \times (S * T)^\lambda)/\equiv \tag{5.38}$$

where $\equiv$ is the transitive closure of $\sim$, where $\sim$ is defined by,

$$\begin{aligned} (a, sw) &\sim (a \cdot s, w), \quad \textit{if } a \in X, s \in S, \\ (a, tw) &\sim (a \cdot t, w), \quad \textit{if } a \in Y, t \in T. \end{aligned} \tag{5.39}$$

Then, $u \in S * T$ acts on Q as determined by

$$(a \otimes w) \cdot u = a \otimes wu. \tag{5.40}$$

Each element of Q can be wirtten as in a canonical form $[a, v]$ where $v = \lambda$ or a shortest member of $S * T$ in canonical form, and a is either

$$\begin{aligned} &a \in X \text{ and } v \text{ does not start with a member of } S, \text{ or,} \\ &a \in Y \text{ and } v \text{ does not start with a member of } T. \end{aligned}$$

Proof. Similar to the proof of Theorem 4, the action is well-defined. Also, $S * T$ acts faithfully on Q. When S and T are nontrivial the proof is similar to Theorem 4 except all 1 s are substitued by λ. Otherwise, if

1. $|X| = |Y| = |S| = |T| = 0$, then, the coproduct is $(\emptyset, \emptyset)$.
2. $|X| = |Y| = |S| = 0$ and $|T| > 0$, then $S * T = T = \{t\}$ where t is an idempotent. Therefore, $S * T$ acts faithfully on $\emptyset \otimes T^\lambda = \emptyset$.
3. $|X| = |S| = |T| = 0$ and $|Y| > 0$, then $S * T = \emptyset$ and it acts faithfully on $Y \otimes \{\lambda\}$.
4. $|X| = |S| = 0$, $|Y| > 0$ and $|T| > 0$. Then, $X \sqcup Y \otimes (S * T)^\lambda = Y \otimes T^\lambda \cong Y$. Therefore, the coproduct is isomorphic to (Y, T) which is faithful.
5. $|X| = |T| = 0$, $|Y| > 0$ and $|S| > 0$. Then, $|S| = 1$ and the coproduct is $(Y \otimes S^\lambda, S)$ which is trivially faithful.
6. $|X| = 0$, $|Y| > 0$, $|S| > 0$ and $|T| > 0$, then the coproduct is isomorphic to $(Y \otimes (S * T)^\lambda, S * T)$ where $S = \{s\}$. To show the coproduct is faithful, we consider the following cases where $u \neq u'$. First, if $u = sw$ where $w = \lambda$ or starts with $t \in T$ and $u' = sw'$ where $w' = \lambda$ or starts with $t' \in T$. Then, take any $y \neq y_0 \in Y$, therefore,

   $$[y, \lambda] \cdot u = [y, sw] \neq [y, sw'] = [y, \lambda] \cdot u'.$$

   Second, if $u = tw$ where $w = \lambda$ or starts with $s \in S$ and $u' = t'w'$ where $w' = \lambda$ or starts with $s \in S$. Then, take any $y \in Y$, therefore,

   $$[y, s] \cdot u = [y, stw] \neq [y, st'w'] = [y, s] \cdot u'.$$

   Third, if $u = sw$, $u' = t'sw''$ where $w \neq w''$, therefore $sw \neq sw''$. Take any $y \in Y$, then,

   $$[y, \lambda] \cdot u = [y, sw] \neq [y \cdot t', sw''] = [y, \lambda] \cdot u'.$$

   Forth, if $u = sw$, $u' = t'sw$, then take any $y \in Y$,

   $$[y, s] \cdot u = [y, s^2 w] = [y, sw] \neq [y, st'sw] = [y, s] \cdot u'.$$

Therefore the action is faithful. Also, the proof for existence of unique morphism that makes the coproduct diagram commute is similar except that the state morphism $\varphi^{State} \colon Q \to Z$ is defined as follows:

$$a \otimes w \mapsto \begin{cases} j_{(X,S)}(a), & \text{if } a \in X, w = \lambda, \\ j_{(Y,T)}(a), & \text{if } a \in Y, w = \lambda, \\ j_{(X,S)}(a) \cdot \varphi^{Operator}(w), & \text{if } a \in X, w \neq \lambda, \\ j_{(Y,T)}(a) \cdot \varphi^{Operator}(w), & \text{if } a \in Y, w \neq \lambda. \end{cases}$$

□

Theorem 9 (Coproducts of Pointed Transformation Semigroups). *Let (X, S) and (Y, T) be pointed transformation semigroups (except $|X| = |Y| = |S| = |T| = 1$). Then, the coproduct is given by the natural inclusions (X, S) and (Y, T) in $(Q, S * T)$ where the coproduct state Q is given by,*

$$((X \vee Y) \times (S * T)^\lambda)/\equiv \tag{5.41}$$

where $\equiv$ is the transitive closure of $\sim$, where $\sim$ is defined by,

$$\begin{aligned} (x_0, w) &\sim (y_0, w), && \textit{if } x_0, y_0 \textit{ are the base-points of } X \textit{ and } Y, \textit{respectively,} \\ (a, sw) &\sim (a \cdot s, w), && \textit{if } a \in X, s \in S, \\ (a, tw) &\sim (a \cdot t, w), && \textit{if } a \in Y, t \in T. \end{aligned} \tag{5.42}$$

The base-point of Q is the equivalence class $x_0 \otimes \lambda = y_0 \otimes \lambda$. Then, $u \in S * T$ acts on Q as determined by

$$(a \otimes w) \cdot u = a \otimes wu. \tag{5.43}$$

Then, each element of $(X \vee Y) \otimes (S * T)$ can be written as in a canonical form $[a, w]$ where $w = \lambda$ or a shortest nontrivial member of $S * T$ in canonical form, and a is either

$$a \in X \setminus \{x_0\} \text{ and } w \text{ does not start with an element of } S, \text{ or,}$$
$$a \in Y \setminus \{y_0\} \text{ and } w \text{ does not start with an element of } T$$

Proof. The proof is similar to the proof of Theorem 5, just we address the cases that are different. To see $S * T$ acts faithfully on Q, when $|X| > 1$ and $|Y| > 1$, the proof is similar to Theorem 4 except all 1 s in the second component of the states must be replaced by the empty string λ. Otherwise if

1. $|X| = |Y| = 1$ and $S = T = \emptyset$, then $Q = \{(*, \lambda)\}$ and the coproduct is $(Q, \emptyset)$ which is trivially faithful.
2. $|X| = |Y| = 1$, $S = \emptyset$ and $T \neq \emptyset$. Then, since T acts faithfully on Y, $|T| = 1$. Let $T = \{t\}$, therefore, the coproduct is $([*, \lambda], \{t\})$, which is faithful.
3. $|X| = 1$, $|Y| > 1$ and $S = T = \emptyset$, then $X \vee Y = \{x_0\} \vee Y \cong Y$. Therefore $S * T = \emptyset$ acts faithfully on $Y \otimes \{\lambda\}$.
4. $|X| = 1$, $|Y| > 1$, $S = \emptyset$ and $T \neq \emptyset$, then $X \vee Y \cong Y$ and $Q \cong Y \otimes T^\lambda$ which is in natural correspondence to Y, i.e. the coproduct is isomorphic to (Y, T). Therefore it is faithful.
5. $|X| = 1$, $|Y| > 1$, $S \neq \emptyset$ and $T = \emptyset$, then $|S| = 1$, $S * T = S$ and $X \vee Y \cong Y$. Therefore, the coproduct is isomorphic to $(Y \otimes S^\lambda, S)$ which is trivially faithful since $|S| = 1$.
6. $|X| = 1$, $|Y| > 1$, $S \neq \emptyset$ and $T \neq \emptyset$, then the coproduct is isomorphic to $(Y \otimes (S * T)^\lambda, S * T)$ where $S = \{s\}$. To show the coproduct is faithful, we consider the following cases where $u \neq u'$. First, if $u = sw$ where $w = \lambda$ or starts with $t \in T$ and $u' = sw'$ where $w' = \lambda$ or starts with $t' \in T$. Then, take any $y \neq y_0 \in Y$, therefore,
$$[y, \lambda] \cdot u = [y, sw] \neq [y, sw'] = [y, \lambda] \cdot u'.$$
Second, if $u = tw$ where $w = \lambda$ or starts with $s \in S$ and $u' = t'w'$ where $w' = \lambda$ or starts with $s \in S$. Then, take any $y \neq y_0 \in Y$, therefore,
$$[y, s] \cdot u = [y, stw] \neq [y, st'w'] = [y, s] \cdot u'.$$
Third, if $u = sw$, $u' = t'sw''$ where $w \neq w''$, therefore $sw \neq sw''$. Take any $y \neq y_0 \in Y$, then,
$$[y, \lambda] \cdot u = [y, sw] \neq [y \cdot t', sw''] = [y, \lambda] \cdot u'.$$
Forth, if $u = sw$, $u' = t'sw$, then take any $y \neq y_0 \in Y$,
$$[y, s] \cdot u = [y, s^2 w] = [y, sw] \neq [y, st'sw] = [y, s] \cdot u'.$$

Therefore the action is faithful. Also, the proof for existence of unique morphism that makes the coproduct diagram commute is similar except that the state morphism $\varphi^{State} \colon Q \to Z$ is defined as follows:

$$[a, w] \mapsto \begin{cases} *_Z & \text{if } a \in \{*\}, w = \lambda \\ *_Z \cdot \varphi^{Operator}(w) & \text{if } a \in \{*\}, w \neq \lambda \\ j_{(X,S)}(a), & \text{if } a \in X, w = \lambda, \\ j_{(Y,T)}(a), & \text{if } a \in Y, w = \lambda, \\ j_{(X,S)}(a) \cdot \varphi^{Operator}(w), & \text{if } a \in X, w \neq \lambda, \\ j_{(Y,T)}(a) \cdot \varphi^{Operator}(w), & \text{if } a \in Y, w \neq \lambda, \end{cases}$$

and the natural inclusions are, $i_X : (X, S) \to ((X \vee Y) \otimes (S * T)^\lambda, S * T)$ maps $x \mapsto x \otimes \lambda$, $s \mapsto s \in S * T$, and $i_Y : (Y, T) \to ((X \vee Y) \otimes (S * T), S * T)$ maps $y \mapsto y \otimes \lambda$, $t \mapsto t \in S * T$. $\square$

Remark 9. If the pointed transformation semigroups are reachable from the basepoints, their coproduct also is reachable. This is true for pointed permutation groups and transformation monoids.

Remark 10. If (X, G) and (Y, H) are permutation groups (resp. transformation monoids), their coproduct in the category transformation semigroups has the semigroup free-product of G and H acting which is not isomorphic the free product of G and H as groups (resp. monoids), as it has no identity element and does not identify the idenitities of G and H. So the coproduct as permutation groups (resp. transformation monoids) is not isomorphic to their coproduct as transformation semigroups.

Similarly for pointed permutation groups (resp. pointed transforamtion monoids).

However, the coproduct of permutation groups in the category of transformation monoids is isomorphic to their coproduct as permutation groups.

5.5.8 Partial Transformation Semigroups

Theorem 10 (Coproducts of Partial Transformation Semigroups). *Let (X_i, S_i) be partial transformation semigroups for each i in some index set I. (NB: in particular, some or all of the (X_i, S_i) may be fully defined!). Then*

$$\coprod(X_i, S_i) = (\bigsqcup X_i, \bigvee S_i) \tag{5.44}$$

is their coproduct, where $\bigsqcup X_i$ is the disjoint union of sets and $\bigvee S_i$ is the semigroup generated by partial transformations s on $\bigsqcup X_i$ such that s agrees with some $s_i \in S_i$ for some $i \in I$ on X_i, and is undefined on the complement of X_i. That is, the action of elements is

$$x \cdot s = \begin{cases} x \cdot s & \text{if } x \in X_i,\ s \in S_i \\ \text{undefined} & \text{otherwise} \end{cases} \tag{5.45}$$

and multiplication of semigroup elements is

$$ss' = \begin{cases} ss' \in S_i & s, s\ \in S_i, \\ \text{undefined} & \text{otherwise.} \end{cases} \tag{5.46}$$

(Note that $x \cdot s$ might not be defined and ss' might be empty in the first cases of both equations above.)

Proof. For all $i \in I$, one has inclusion partial transformation semigroup morphisms $\iota_i \colon (X_i, S_i) \to (\bigsqcup X_i, \bigvee S_i)$ such that if $j_i \colon (X_i, S_i) \to (Q, T)$ are morphisms for some fixed partial transformation semigroup (Q, T), then there is a unique morphism $\varphi \colon (\bigsqcup X_i, \bigvee S_i) \to (Q, T)$ given by defining for $x \in \bigsqcup_{i \in I} X_i$, where $x = x_i$, that $\varphi(x_i) = j_i(x_i)$ and for $s \in \bigvee S_i \setminus \{\emptyset\}$, with s agreeing on X_i with $s_i \in S_i$, that $\varphi(s) = j_i(s_i)$. Any other member of $\bigvee S_i$ must be the empty transformation (which is not in the domain of $\varphi^{Operator}$). Clearly, φ is a morphism. Then we have $j_i = \varphi \circ \iota_i$ holds for all i. Moreover, φ is unique since the equation says $\varphi(x_i) = \varphi(\iota_i(x_i)) = j_i(x_i)$, and, similarly for the nonempty semigroup elements in $\bigvee S_i$, uniquely determining φ. $\square$

Remark 11. Always $\bigvee S_i$ will be contained in the formal disjoint union of the $S_i \setminus \{\emptyset\}$ union the singleton $\{\emptyset\}$.

Remark 12. If (X, S) is a partial transformation semigroup and the empty transformation is *not* in S, then $(X, S \cup \{\emptyset\})$ is isomorphic to (X, S) in the category PTS.

Proof. Map the set X in each direction by the identity map. Map in each direction the semigroups minus the empty transformation by the identity map on S, then the compositions are the identity morphisms. $\square$

For partial transformation monoids and partial permutation groups, the analogous construction of coproduct holds.

5.6 Coproduct of Automata

A **partial deterministic automaton** is a triple $\mathcal{A} = (Q, q_0, X, \delta)$ consisting of two sets: Q and X, an element of Q, q_0 and a partial function $\delta\colon Q \times X \to Q$. If δ is a function, i.e., $\delta(q, x)$ always has exactly one element for all $q \in Q$ and $x \in X$ then $\mathcal{A}$ is called a **fully-defined** or **complete deterministic automaton**. If $\delta(q, x)$ always has *at most one* element, then $\mathcal{A}$ is called **deterministic**. If $\delta(q, x)$ does not have any elements then we say $\delta(q, x)$ is undefined. The case of general δ, one calls *partial, non-deterministic* even for the special cases of deterministic or fully-defined deterministic automata.

The set Q is called the set of **states**, q_0 the initial state, X the **input alphabet** (and its members $x \in X$, **inputs** or **input letters**), and δ the **transition function**. Denote $\delta(q, x)$ by $q \cdot x$ for brevity where $q \in Q, x \in X$, and extend this notation to subsets $W \subseteq Q$ by $W \cdot x = \bigcup_{w \in W} w \cdot x$. Similarly, if $f\colon X \to Y$ is a partial multivalued function, or equivalently $f\colon X \to \mathcal{P}(Y)$ is a function, then we define $f(W) = \bigcup_{w \in W} f(w)$ where $W \subseteq X$. Also, in case $\delta(q, x)$ is a singleton $\{x'\}$, we shall write $\delta(q, x) = x'$ for notational convenience. Similarly for a general multivalued partial function f, if $f(x)$ is a singleton $\{y\}$, then we write $f(x) = y$.

Thus we have: An automaton $\mathcal{A}$ is complete if $|q \cdot x| \geq 1$ for all states $q \in Q$ and inputs $x \in X$.
$\mathcal{A}$ is deterministic if $|q \cdot x| \leq 1$ for all states $q \in Q$ and inputs $x \in X$.
So $\mathcal{A}$ is complete deterministic if $|q \cdot x| = 1$ for all states $q \in Q$ and inputs $x \in X$.

$\mathcal{A}\mathbf{utom}^{\mathbf{det}}$ and $\mathcal{A}\mathbf{utom}^{\mathbf{det}}_{\mathbf{(c)}}$, consist of all partial deterministic automata, and all complete deterministic automata, respectively. In each case, a morphism $\varphi\colon \mathcal{A} \to \mathcal{A}'$ is defined as a pair $\varphi = (\varphi^{State}\colon Q \to Q', \varphi^{Input}\colon X \to X')$ such that

$$\begin{aligned} \varphi^{State}(\delta(q, x)) &\subseteq \delta'(\varphi^{State}(q), \varphi^{Input}(x)), \text{ and,} \\ \varphi^{State}(q_0) &\subseteq \varphi^{State}(q_0'). \end{aligned} \tag{5.47}$$

Here φ^{State} and φ^{Input} are functions (in particular, these are fully defined and single-valued), and composition of morphisms is component-wise composition of functions. Note that equation (5.47) asserts a subset relation of two subsets of the state set, where we regard the left hand side as the empty set whenever $\delta(q, x)$ is undefined. In the case of deterministic automata, the right hand side can have at most one element. In the fully defined deterministic case, both sides of (5.47) refers to a single state of $\mathcal{A}'$.

Remark 13. If $\varphi\colon (Q, I, X, \delta) \to (Q', I', X', \delta')$ is an $\mathcal{A}utom_S$ morphism, when $w = x_1 \cdots x_n \in X^*$ by $\varphi^{Input}(w)$ we mean the word $\varphi^{Input}(x_1) \cdots \varphi^{Input}(x_n) \in X'$. Also, $\delta^*(q, wa) = \bigcup_{q' \in \delta^*(q,w)} \delta(q', a)$ where w is not the empty word.

It is common to use automata having a unique initial state and we now restrict to the subcategory of $\mathcal{A}utom_S$ consisting of such automata. This forces one to identify initial states in the coproduct. The structure of coproducts of automata appears to have been first studied by A. Wiweger [50], and, more comprehensively, by H. Ehrig [16] in various categories. The latter describes the coproduct as "*much more complicated*" when, as in our Theorems 11 and 13, the automata are permitted to have different input alphabets (as well as different output alphabets in Theorem 13), and as *"seem[ing ....] rather "uncanonical" "* for the complete deterministic cases characterized here. Using the tensor product notation as in our treatment of the coproduct of pointed transformation semigroups and pointed permutation groups (Section 5.5), the coproduct of deterministic complete automata (with or without output) can be described more concisely and intuitively.

Theorem 11 (Coproduct for Complete Deterministic Automata with Initial State). *Let $\mathcal{A} = (Q_A, q_A, X_A, \delta_A)$ and $\mathcal{B} = (Q_B, q_B, X_B, \delta_B)$ be two complete deterministic automata. Then their coproduct is*

$$\amalg = ((Q_A \vee Q_B) \otimes ({X_A}^+ * {X_B}^+)^\lambda, \{*\}, X_A \sqcup X_B, \delta),$$

where $Q_A \vee Q_B$ is the pointed union of the state sets identifying the base points with action just like in our construction for transformation semigroups (Theorem 9), i.e. rewriting this, the states are $(Q_A \vee Q_B) \otimes (X_A \sqcup X_B)^*$ where a letter from X_A acts on Q_A like in the 1st automaton $\mathcal{A}$, a letter from X_B acts on Q_B like in the 2nd automaton $\mathcal{B}$, in all other cases the letter is appended to give a new state.

Proof. The natural inclusion $i_{\mathcal{A}} \colon \mathcal{A} \to \amalg$ is defined as follows:

$$\begin{aligned} i_{\mathcal{A}}^{State} \colon Q_A &\to (Q_A \vee Q_B) \otimes ({X_A}^+ * {X_B}^+)^\lambda \\ q &\mapsto q \otimes \lambda, \\ i_{\mathcal{A}}^{Input} \colon X_A &\to X_A \sqcup X_B \\ x &\mapsto x, \end{aligned} \tag{5.48}$$

The function $i_{\mathcal{A}}$ is a well-defined automata morphism. Indeed, for every $q \in Q_A$ and $x \in X_A$,

$$\begin{aligned} i_{\mathcal{A}}^{State}\left(\delta_A(q, x)\right) &= \delta_A(q, x) \otimes \lambda \\ &= q \otimes x \\ &= \delta\left(q \otimes \lambda, x\right) \\ &= \delta\left(i_{\mathcal{A}}^{State}(q), i_{\mathcal{A}}^{Input}(x)\right). \end{aligned}$$

The natural inclusion $i_{\mathcal{B}} : \mathcal{B} \to \amalg$ is defined similarly. Supposing $j_{\mathcal{A}} \colon \mathcal{A} \to \mathcal{Z} = (Q_Z, q_Z, X_Z, \delta_Z)$ and $j_{\mathcal{B}} \colon \mathcal{B} \to \mathcal{Z}$ are two $\mathcal{A}\mathbf{utom}^{\mathbf{det}}_{\mathbf{(c)}}$ morphisms, it is shown that there is a unique $\mathcal{A}\mathbf{utom}^{\mathbf{det}}_{\mathbf{(c)}}$ morphism $\varphi = (\varphi^{State}, \varphi^{Input})$ which makes the following diagram commute.

$$\begin{tikzcd}
\mathcal{A} \arrow[dr, "i_{\mathcal{A}}"] \arrow[ddr, bend right, "j_{\mathcal{A}}"'] & & \mathcal{B} \arrow[dl, "i_{\mathcal{B}}"'] \arrow[ddl, bend left, "j_{\mathcal{B}}"] \\
& ((Q_A \vee Q_B) \otimes ({X_A}^+ * {X_B}^+)^\lambda, \{*\}, X_A \sqcup X_B, \delta) \arrow[d, dashed, "\varphi"] & \\
& \mathcal{Z} = (Q_Z, q_Z, X_Z, \delta_Z) &
\end{tikzcd} \tag{5.49}$$

The existence of a unique $\varphi^{Input} : X_A \sqcup X_B \to X_Z$ making the input letter component commute is guaranteed by the fact that $X_A \sqcup X_B$ is the coproduct of X_A and X_B as sets.

The function $\varphi^{State}\colon (Q_A \vee Q_B) \otimes ({X_A}^+ * {X_B}^+)^\lambda \to Q_Z$ is defined by

$$q \otimes w \mapsto \begin{cases} q_Z, & \text{if } q \otimes w = *, \\ j_{\mathcal{A}}^{State}(q), & \text{if } q \in Q_A \text{ and } w = \lambda, \\ j_{\mathcal{B}}^{State}(q), & \text{if } q \in Q_B \text{ and } w = \lambda, \\ \delta_Z^+ \left(j_{\mathcal{A}}^{State}(q), \varphi^{Input}(w_1) \cdots \varphi^{Input}(w_n) \right), & \text{if } q \in Q_A \text{ and } w \neq \lambda, \\ \delta_Z^+ \left(j_{\mathcal{B}}^{State}(q), \varphi^{Input}(w_1) \cdots \varphi^{Input}(w_n) \right), & \text{if } q \in Q_B \text{ and } w \neq \lambda, \end{cases} \tag{5.50}$$

where $w = w_1 \cdots w_n$ and $w_i \in X_A \sqcup X_B$. The function φ^{State} is well-defined. Well-definedness of the state map is similarly established as in Theorem 9. Next we show φ is an $\mathcal{A}$utom morphism: Let $q \in Q_A$ and $x \in X_A \sqcup X_B$,

$$\begin{aligned} \varphi^{State}(\delta(q \otimes w, x)) &= \varphi^{State}(q \otimes wx) \\ &= \delta_Z^+ \left(j_{\mathcal{A}}^{State}(q), \varphi^{Input}(w_1) \cdots \varphi^{Input}(w_n) \varphi^{Input}(x) \right) \\ &= \delta_Z \left(\delta_Z^+ \left(j_{\mathcal{A}}^{State}(q), \varphi^{Input}(w_1) \cdots \varphi^{Input}(w_n) \right), \varphi^{Input}(x) \right) \\ &= \delta_Z(\varphi^{State}(q \otimes w), \varphi^{Input}(x)). \end{aligned} \tag{5.51}$$

Also, $\varphi^{State}(i_{\mathcal{A}}(q)) = \varphi^{State}(q \otimes \lambda) = j_{\mathcal{A}}^{State}(q)$. These calculations are the same if $q \in Q_B$ but using $j_{\mathcal{B}}^{State}$ instead of $j_{\mathcal{A}}^{State}$.

Therefore φ makes Diagram 5.49 commute. If there is another morphism φ_2 for which Diagram 5.49 commutes, then for every $q \in Q_{\mathcal{A}}$, using uniqueness of φ^{Input} (i.e., $\varphi_2^{Input} = \varphi^{Input}$), we have for all $w \in (X_A \sqcup X_B)^*$,

$$\begin{aligned} \varphi_2^{State}(q \otimes w) &= \varphi_2^{State}(\delta^+(q \otimes \lambda, w)) \\ &= \delta_Z^+(\varphi_2^{State}(q \otimes \lambda), \varphi^{Input}(w_1) \cdots \varphi^{Input}(w_n)) \\ &= \delta_Z^+(\varphi_2^{State}(i_{\mathcal{A}}^{State}(q)), \varphi^{Input}(w_1) \cdots \varphi^{Input}(w_n)) \\ &= \delta_Z^+ \left(j_{\mathcal{A}}^{State}(q), \varphi^{Input}(w_1) \cdots \varphi^{Input}(w_n) \right) \\ &= \varphi^{State}(q \otimes w). \end{aligned} \tag{5.52}$$

The case of $q \in Q_B$ is similar using $i_{\mathcal{B}}^{State}$ and $j_{\mathcal{B}}^{State}$. It follows $\varphi_2^{State} = \varphi^{State}$, so we conclude $\varphi = \varphi_2$. □

We remark that the semigroup of the coproduct of automata is the free semigroup on the disjoint union of their input alphabets, as is easy to see by considering that input letters act on most states essentially by concatenation.

Theorem 12 (Coproduct for Partial Deterministic Automata with Initial State). *Let $\mathcal{A} = (Q_A, q_A, X_A, \delta_A)$ and $\mathcal{B} = (Q_B, q_B, X_B, \delta_B)$ be two partial (deterministic) automata. Then their coproduct is $(Q_A \vee Q_B, q, X_A \sqcup X_B)$, with the same states as the coproduct of pointed partial transformation semigroups, and action*

$$\delta(q, a) = \begin{cases} \delta_A(q, a) & \text{if } q \in Q_A \text{ and } a \in X_A \\ \delta_B(q, a) & \text{if } q \in Q_B \text{ and } a \in X_B \\ \emptyset & \text{otherwise, i.e. undefined.} \end{cases}$$

Here q_A and q_B are identified in $Q_A \vee Q_B$.

Note that the coproduct of complete automata (resp. transformation semigroups or permutation groups) taken in the category of partial automata (resp. partial transformation semigroups) is very different in structure from their coproduct in the category of complete automata (resp. transformation semigroups or permutation groups). In particular, the category in the partial categories preserves finiteness, but this is rarely the case for the non-partial case.

For non-deterministic automata the coproduct is similar to the partial deterministic case, with letters acting only on states where their actions were defined in the component automata.

Theorem 13 (Coproduct for Complete Deterministic Automata with Outputs with Initial State (Mealy Automata)). *Let $\mathcal{A}_1 = (Q_1, q_1, X_1, Y_1, \delta_1, \epsilon_1)$ and $\mathcal{A}_2 = (Q_2, q_2, X_2, Y_2, \delta_2, \epsilon_2)$, be two complete deterministic automata with transition functions $\delta_i : Q_i \times X_i \to Q_i$ and output functions $\epsilon_i : Q_i \times X_i \to Y_i$ mapping states and input letters to output letters. Then their coproduct is*

$$\amalg = ((Q_1 \vee Q_2) \otimes ({X_1}^+ * {X_2}^+)^\lambda, \{*\}, X_1 \sqcup X_2, Y, \delta, \epsilon),$$

where $Q_1 \vee Q_2$ is the pointed union of the state sets identifying the base points with action exactly as in our construction for automata (Theorem 11), i.e. rewriting this, the states are $(Q_1 \vee Q_2) \otimes (X_1 \sqcup X_2)^*$ where a letter from X_i acts on Q_i like in the ith automaton $\mathcal{A}_i$ ($i \in \{1, 2\}$), in all other cases the letter is appended to give a new state. Let $Q^{new} = ((Q_1 \vee Q_2) \otimes (X_1 \sqcup X_2)^*) \setminus ((Q_1 \vee Q_2) \otimes \lambda)$, i.e., the 'new' states that are not in the image of the inclusion maps from the $\mathcal{A}_i$. The output set Y is $Y_1 \sqcup Y_2 \sqcup Q^{new}$. The output function $\epsilon : ((Q_1 \vee Q_2) \otimes (X_1 \sqcup X_2)^*) \times (X_1 \sqcup X_2) \to Y$, is given by

$$\epsilon(q \otimes w, x) = \begin{cases} \epsilon_i(q', x) & \text{if } q \otimes w \in (Q_1 \vee Q_2) \otimes \lambda, q \otimes w = q' \otimes \lambda, q' \in Q_i, x \in X_i \ (i \in \{1, 2\}) \\ q' \otimes x & \text{if } q \otimes w \in (Q_1 \vee Q_2) \otimes \lambda, q \otimes w = q' \otimes \lambda, q' \in Q_i, x \in X_j \ i \neq j \\ q \otimes wx & \text{if } q \otimes w \notin (Q_1 \vee Q_2) \otimes \lambda \end{cases}$$

Proof. The proof is just as for Theorem 11, but for the output function the unique mapping is defined in the only way possible, which one verifies works to give a morphism of Mealy automata. Indeed, let the complete deterministic Mealy automaton $\mathcal{Z} = (Q_Z, q_Z, X_Z, Y_Z, \delta_Z, \epsilon_Z)$ be given and $j_{\mathcal{A}_i} : \mathcal{A}_i \to \mathcal{Z}$, $i \in \{1, 2\}$ be two arbitrary $\mathcal{M}\mathbf{ealy}\mathcal{A}\mathbf{utom}^{\mathbf{det}}_{\mathbf{(c)}}$ morphisms which make the coproduct diagram commute (similar to Diagram 5.49). Then, according to Theorem 11 there is unique morphism $(\varphi^{State}, \varphi^{Input})$ which makes the coproduct diagram commute. Also, $\varphi^{Output} : Y \to Y_Z$ is defined as follows:

$$y \mapsto \begin{cases} j^{Output}_{\mathcal{A}_i}(y_i), & \text{if } y = y_i \in Y_i, \\ \epsilon_Z(\varphi^{State}(q \otimes w'), \varphi^{Input}(x)) & \text{if } y = q \otimes w'x. \end{cases} \tag{5.53}$$

□

Thus, input symbols from a component applied a state of that component (in the embeded copy in the coproduct) yields the same output as for that component. But, as soon as, an input letter would take one to a 'new' state (not equivalent to one of the form $q' \otimes \lambda$), the output merely returns the new state, which uniquely determines the start and the input symbol, since the new state is obtained essentially by appending the new letter onto the old state.

Chapter 6

Conclusion

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