

THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

Shapes and games

—Reshaping distributions and images via ODEs

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Abstract. This thesis summarizes the four articles *Decisions and disease*, *Diversity strengthens competing teams*, *Shape analysis via gradient flows on diffeomorphism groups* and *Team game adaptive dynamics*. Each article has a different context, but the mathematical aims are unified as we prove optimality of solutions or well-posedness of dynamics. Moreover, the modeling perspective is central to each investigation. In *Decisions and disease* we combine the classic SIR and SIS models from epidemiology with the prisoner's dilemma game. Here, the steady state solutions are interpreted in terms of cooperation during a pandemic. Another game is studied in *Diversity strengthens competing teams*, namely the so-called Game of Teams, for which all Nash equilibria are found. The optimal solutions, i.e., the Nash equilibria, are characterized by teams with maximal diversity in the sense that the successful teams have as different members as possible. Gradient flows are explored next, with a focus on an efficient method for image matching. We prove well-posedness of a gradient flow that is regularized by the deformation of the Riemannian metric of the manifold which the images are defined on. Lastly, the adaptive dynamics framework is applied to the Game of Teams. This model of evolution pushes the strategies of the game in the direction of the selection gradient. We have analyzed the well-posedness of the adaptive dynamics equations and answered questions about the stationary solutions, that is which solutions that do not display any dynamics despite the selection pressure that the selection gradient forces on them. It is found that the stationary solutions agree with the Nash equilibria.

Keywords: game theory, prisoner's dilemma, equilibrium strategy, disease, compartmental model, epidemiological model, shape analysis, differential equations, differential geometry

List of publications

This thesis is based on the work contained in the following papers and manuscripts:

Paper I: Karlsson, C. & Rowlett, J. (2020). Decisions and disease: a mechanism for the evolution of cooperation. *Nature Scientific Reports*, 10(1), p 13113, <https://doi.org/10.1038/s41598-020-69546-2>

Paper II: Rowlett, J., Karlsson, C. & Nursultanov, M. (2021). Diversity strengthens competing teams. *Royal Society Open Science* 9(8), p 211916, <https://doi.org/10.1098/rsos.211916>

Paper III: Balehowsky, T., Karlsson, C. & Modin, K. (2023). Shape analysis via gradient flows on diffeomorphism groups. *Nonlinearity* 36(2), pp 862-877, <https://doi.org/10.1088/1361-6544/aca73c>

Paper IV: Karlsson, C., Gerlee, P. & Rowlett, J. (2024). Team game adaptive dynamics. *Submitted*. arXiv:2401.17090

Author contribution:

Paper I: I scanned the literature, finding the connection between the SIR model and the dynamic parameter β , contributed to writing the manuscript, and I did the numerical study as well as many of the pen-and-paper calculations.

Paper II: I did many of the pen-and-paper calculations, especially on the discrete game, and I contributed to the literature study and on writing the manuscript.

Paper III: I computed some of the important equations, and I contributed to the analysis and the manuscript writing.

Paper IV: Based on the suggestion of P. Gerlee to use adaptive dynamics and the ideas from game theory of J. Rowlett, I formalized the adaptive dynamics framework in the current context, wrote examples and code, did most of the analysis and drafted a first manuscript. In all publications, I continuously improved the manuscripts.

Acknowledgements

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Carl-Joar

Göteborg, 2024

Notation, abbreviations and nomenclature

$\mathbb{Z}$	The integers ..., -2 , -1 , 0 , 1 , 2 , ...
$\mathbb{R}$	The real numbers
$\mathbb{C}$	The complex numbers
$\mathfrak{X}(M)$	The space of smooth vector fields on a manifold M
g	Riemannian metric
$\mathfrak{g}$	Lie algebra
a.e.	Almost Everywhere
game	A collection of players, payoff functions and strategies
E	Expectation, see §4.1; energy, see §5.1
p	Expectation of normalized strategies, payoff
CA	Competitive Ability
MCA	Mean Competitive Ability
C	The upper bound on MCAs; the cost in Donor-Recipient games
SIR	A compartment model with categories susceptible, infectious and removed
SIS	A compartment model with categories susceptible and infectious. Typically, this models a disease without immunity.
A	Either the adaptive dynamics mapping, or the inertia operator. There should be no risk for confusion; the inertia operator only appears in the Lie group context.
∇E	The selection gradient, see §4.1.4; the gradient of the energy functional, see §5.1

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Introduction

I'm stepping through the door
And I'm floating in a most peculiar way
And the stars look very different today
—David Bowie (in *Space Oddity*)

The importance of modeling natural phenomena, societies, complex systems, etc. cannot be overstated. In order to understand the world, it is helpful to reduce the level of detail, keeping the essential mechanisms at the core of the model. For example, Newton's theory of gravity can be used to understand the motion of satellites and also how to launch satellites into orbit. The theory explains the force which is needed for the launch and why launching sites are usually close to the equator of the Earth [18]. However, classical mechanics alone cannot explain why clocks on satellites are out of sync with clocks on Earth's surface. The theory of relativity has been necessary in order to solve the synchronization problem, and understanding the relativistic effects on satellites has been crucial for the global positioning system (GPS) [3]. This does not mean that Newtonian mechanics is wrong. Instead, the situation is a reminder that every model of nature is a simplification with limitations. The effects of relativity become apparent at high speeds when there are several observers measuring time or position in different directions in spacetime [29]. Newton's mechanics is still extremely useful in the right context, and moreover, it highlights the essential interplay between force and motion. If general relativity had been necessary to understand the motion of “slow”

objects, such as animals and trains, we would have a lot of trouble using the theory. Einstein [22] said it wisely: “It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience.”

Another scientist who emphasized the idea of modeling principles was von Neumann, claiming [66] that truth “is much too complicated to allow anything but approximations” but as he was also a strong advocate of using the mathematics toolbox, contributing to the development of the mathematical economics theory during the 1940’s and the early 1950’s. In 1944, von Neumann and Morgenstern published their book *Theory of Games and Economic Behaviour* [76], which is considered to have started the interdisciplinary research field of game theory. Naturally, games had been discussed and solved in mathematical contexts long before 1944, with records going back to ancient times [69], but it was the *Theory of Games and Economic Behaviour* that established the formalism of mathematical game theory that we are used to seeing today. Here, strategic decisions were analyzed under the assumption that players are rational in the sense that they strive to maximize their individual payoff in the game at hand. The payoff (which is quantified in currency, for example) is determined by the rules of the game and the players’ collected choices of strategies. Some of the basic games that were understood during these times highlighted the mechanisms of trading and negotiation, which to some extent lacked the concise and quantitative analysis that game theory provided.

Later during the 1900s, games were used to analyze phenomena in ecology by re-interpreting the payoff to players in games as survival benefits. Attempts were made to explain animal conflicts between members of the same species as games that are repeated (as such animal conflicts usually repeat in nature) and in that context, each strategy’s popularity was developing over time such that the more successful strategies increase in popularity. The changing popularity of certain strategies was interpreted as an evolutionary process, namely the evolution and/or spreading of phenotypes in animal populations.

Today, game theory analysis is an essential part of modern decision-making. Agreements such as the Kyoto protocol (on reducing the climate footprint worldwide) undergo game theory analysis. Economy, negotiation, trade, resource management, ecology and physics are just some examples of applications of the modern game theory that was formalized during the 20th century [53].

Mathematics provides methods to discover structures and processes in phenomena or ideas. Game theory highlighted how cooperation is dependent on the payoff balance, that is how much advantage certain choices give compared to making other decisions, for instance. Another field of mathematics that has advanced our understanding of the structures of phenomena is mechanics. First founded by Isaac Newton in the 17th century, the laws of mechanics were hidden in latin and geometric notation. The first translation to French, by Émilie du Châtelet, which she finalized on hospital and which was posthumously published in 1756, used the modern mathematical language of differentials to describe the force laws [60, 6]. Only a few years later, Italian-French mathematician and astronomer Joseph-Louis Lagrange re-formulated the Newtonian mechanics: the motion of objects are seen as extreme paths of an energy function that is defined on a configuration space. This new perspective adds a layer of understanding. For instance, light rays could be seen to take the path that minimizes the time it takes from the light source to the observation point. The trajectory is in this sense optimal. Einstein did also recognize the generalizations of Newton's theory in his theory of general relativity, noting that a weak gravitational field and slowly moving particles experience the classical potential (the $1/r^2$ law) that Newton formulated [74].

Einstein's theory of gravity emphasized that the standard reference of movement was freely falling particles, rather than "free" particles as in the classical mechanics theory [79]. Consequently, the "old" theory could only be local; a freely falling particle in New Zealand is a different reference compared to a freely falling particle in Scandinavia, yet both situations are bounded by the same physical laws. The physical laws have to transform geometrically. And not just that: Einstein realized that physical objects influence the geometry. He was the first to understand correctly how

heavy bodies, such as planets, create a curved spacetime. By comparing the apparent positions of stars which appear near the Sun on the sky (in daylight during an eclipse) to their positions as determined at night (when their light does not pass by the Sun), the light deflection that Einstein predicted could be observed. In 1919, the first experimental results confirmed those predictions. These experiments produced the image in Figure 1.1, showing a trace of light that curves around the Sun.

The mathematical framework that made it possible for Einstein and his collaborators² to adequately describe the physical laws of spacetime is *differential geometry*. In short, spacetime is an object with “intrinsic” time and length units, but the observations of time and length depends on the position and movement of the observer. Moreover, gravity distinguishes freely falling particles from others; only the freely falling objects experience a flat spacetime. In spacetime, “flat” roughly means that space is measured against the up, right and forward directions, while time is a separate measurement. On Earth’s surface as well as in many physically relevant situations, however, space and time is not flat. General relativity makes sense of this using a *metric*, that is, a (possibly curved) notion of directions and time, coming from differential geometry. The only way to combine gravity and spacetime geometry is through differential geometry.

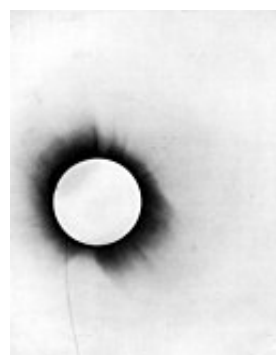


Figure 1.1: Observations of light deflection in 1919.¹

Just shortly after the publication of general relativity in 1915, Einstein and others formulated the laws of spacetime using the formalism that Lagrange initiated in the late 18th century. The Einstein field equations in vacuum, for instance, were discovered to be extreme paths of metrics to

¹Image source: F. W. Dyson, A. S. Eddington, and C. Davidson, “A Determination of the Deflection of Light by the Sun’s Gravitational Field, from Observations Made at the Total Eclipse of May 29, 1919” *Philosophical Transactions of the Royal Society of London. Series A* (1920): 291-333.

²There are still debates over how much Einstein worked together with others, especially his first wife Mileva Marić.

the following integral:

$$S[g] = \int_D R \mu_g,$$

where μ_g is the volume form associated to g , the integral runs over space-time D and R is the spacetime (scalar) curvature [74]. The important note to make is that mathematics that was developed for mechanics now applied to new physical theories. It could reveal new structure. Equations of motion, which were of interest to Newton, Lagrange, Einstein and many others, also had a meaning in the sense of optimality. They were the shortest or fastest or least energy consuming motions. But how could they know which integrals that were relevant? And which equations were they looking for? The answers are usually complicated. In some instances, the equation itself is the “first principle”, the starting point of the theory, while in many – if not most – the leading argument for the theory is the optimality; nature’s objects behave according to “least action” or to minimize energy or maximize entropy.

In some cases, the equations of motions are well-known for a very long time even if no one knows about their “optimality.” The Euler equations of incompressible hydrodynamics, for instance, were one of the first partial differential equations to be written down. They were derived from principles of mass conservation (that is, matter cannot disappear) and Newton’s laws of motion. In the 1960s, Arnold found the optimality principle of these equations: they are the shortest path, measured by a right-invariant metric on the group of diffeomorphisms preserving the volume element of the domain [1]. For a detailed description, see Chapter 5 of this thesis.

One fundamental problem, apart from deriving equations and assert their validity based on physical principles or modeling considerations, is *to solve* the equations. Solving equations might require special techniques or the development of new techniques. In either case, if the equations are solved, there could remain questions about the properties of the solutions. Einstein encountered these problems after publishing the field equations of general relativity. Did the solutions behave physically? In particular, would matter propagate at a speed that is bounded by the speed of light? A number of scientists would spend many years to prove that Einstein’s

field equations admit “nice” solutions. Some of the concerns that Einstein and others were working on had to do with coordinates; it seemed as if the equations could be expressed in two different coordinate systems and separate into different solutions even if they had agreed up until they did not anymore. The solution seemed to be non-unique. After a couple of decades, the problem was resolved by writing the equations as an *initial value problem* [68]. Even if that work required many years of collaborative effort, it was logical; as Isenberg [37] writes: “Ever since Newton’s formulation of particle mechanics over three hundred years ago, one of the most widely used methods of modeling physical systems is via an initial value formulation.” The basic initial value problem, much simpler than what proved that the Einstein equations behaved nicely [24], is usually written as

$$y'(t) = f(y, t), \quad y(0) = y_0, \quad (1.1)$$

where y_0 is the initial data and f describes the rate of change of the solution $y(t)$. In later chapters, such problems will emerge frequently, as there is a very general, deterministic interpretation of the initial value problem: If the current state, y , is known and it is known in which direction it is heading at any time, then the future states can be predicted. At least, that is what every scientist *hopes* that it will do. Considerable effort has been made and is still made to ensure that initial value problems in fact make a single (that is, unique), reliable prediction.³ Initial value problems are at the heart of papers I, III and IV of the current thesis.

Among all ordinary differential equations (ODEs) and initial value problems, the following is probably considered the most basic starting point of the theory:

$$y'(t) = ay(t), \quad y(0) = y_0, \quad (1.2)$$

for some constant a . The unique solution is $y(t) = y_0 e^{at}$, that is, if the rate of change of the value y is proportional to y itself, then the solution is exponential growth (for $a > 0$) or decay (for $a < 0$). It appears, however,

³Even so, if the predictions are reliable and unique, it could still happen that the physical system itself is chaotic. Weather systems are good examples of that.

that this equation limits our world far too much. In particular, based on Newton's laws of motion, it is necessary to write equations that govern the *acceleration* of objects, which is a second order derivative of position with respect to time. That is,

$$y''(t) = F(y, t)$$

would be a very interesting problem. For instance, Hooke's law for springs says that the force is proportional to the spring's extension, $F = -ky$. Combining this with Newton's equations of motion, $y'' = -ky$. In terms of position and velocity, the equations of motion is a pair of equations: one for the position and one for the velocity. Introduce the velocity $v = y'$ and write the equations:

$$\begin{aligned} v' &= -ky \\ y' &= v. \end{aligned}$$

Using matrix notation, as will be described in detail in Chapter 2, Hooke's law gives $\mathbf{y}' = A\mathbf{y}$. That is, the basic form of the initial value problem remains. The solutions get more complex, since there are now two governing equations. However, the criteria that determine if there exist well-behaved solutions are formulated for systems of equations of *any* size just as well as for the one-dimensional problem (1.2). Should the number of equations be very large, the initial value problem could be difficult to analyze from an algebraic point of view, but the idea still relies on the results from the above weight-on-a-spring system. A greater challenge is posed by infinite-dimensional systems. Such systems appear naturally in some modeling situations, such as dynamics of functions or shapes.

This thesis collects three articles that rely on game theory and one article in shape analysis. Mathematicians at the division of applied mathematics will probably argue that these articles are in "pure" mathematics, meaning that they do not involve real-world data and can exist entirely as mathematical investigations. But mathematicians in pure mathematics will probably argue that the articles belong to the applied sciences, since the problems and the analysis are formulated with the real world in mind. I will leave it to the reader to decide on that matter. The two articles *Diversity strengthens*

competing teams and *Decisions and disease: a mechanism for the evolution of cooperation* focus on the question about collaboration between individuals or groups of individuals. Using game theory, they provide examples of how individual-level interaction and collective-level dynamics are interfering with each other. In *Shape analysis via gradient flows on diffeomorphism groups*, we turn to another context. Here, the main question is how it is possible to deform a shape and match it with another shape efficiently. The fourth article, *Team game adaptive dynamics*, is again game theoretical but the attention is on the dynamics of game strategies. This dynamics is driven by the so-called “selection gradient” and it is not very far-fetched to say that the ideas from shape analysis influenced the course of this work.

But what theoretical foundations are these articles based on? In each of the articles, we argue for the existence of certain solutions to problems: The first two articles prove the existence of equilibria, whereas the next two articles prove the existence of a time evolution. The problems that are solved in the articles are related to certain initial value problems or to optimality. Two different initial value problems are solved: The evolution away from an initial strategy and the evolution of shapes that deform towards a “target shape”, for example a rectangle which is stretched and squeezed into the shape of a disc. The next chapter provides a roadmap of the mathematics that lead up to the articles of this thesis.

2

Background: linear algebra, geometry and dynamics

You just take that one road the whole time... I hope they don't get lost. I'm so bad at giving directions.

—Glinda (in *Wicked*, the musical)

This chapter introduces some of the ideas and the theory that underlies the work behind this thesis' articles. It begins with concepts from linear algebra on the Euclidean space and game theory. The next sections sets the notation and explains a few concepts from analysis and geometry. It is not the intent to provide an extensive textbook on these topics, but I believe that a background chapter might help the reader to see the connection between well-established results in mathematics and the results that belong to this thesis. After all, mathematics is a very wide landscape and this chapter should provide directions to make it easier to navigate.

2.1 Linear algebra

Consider a square matrix A with components in the complex numbers. Let I be the identity matrix of size $n \times n$ with ones on the diagonal and zeroes

elsewhere:

$$I = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & & \ddots & 0 \\ 0 & 0 & \dots & 1 \end{bmatrix}.$$

If it acts on a vector in $\mathbb{C}^n$, it leaves the vector unchanged. In other words, it represents the *identity* mapping $\mathbf{y} \mapsto \mathbf{y}$. A vector in $\mathbb{C}^n$,

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix},$$

is called an eigenvector of A if there is a complex-valued number λ such that the equation $A\mathbf{y} = \lambda\mathbf{y}$ has a solution $\mathbf{y}$ which is not a zero vector. Define the kernel of a matrix as the set of vectors $\{\mathbf{y} \in \mathbb{C}^n : A\mathbf{y} = 0\}$, where the 0 is the vector with all components zero. Rewriting $A\mathbf{y} = \lambda\mathbf{y}$ into $(A - \lambda I)\mathbf{y} = 0$, eigenvectors are non-trivial vectors in the kernel space of $A - \lambda I$.

The eigenvalues of a $n \times n$ square matrix A are roots of the polynomial $\det(A - \lambda I)$, which is of degree n . In general, any polynomial p of degree n has q distinct zeroes with $q \leq n$ and can be decomposed as $p(\lambda) = (\lambda - \lambda_1)^{m_1}(\lambda - \lambda_2)^{m_2} \cdot \dots \cdot (\lambda - \lambda_q)^{m_q}$, where each positive integer m_j is called the algebraic multiplicity of the eigenvalue λ_j . Then, $\sum_{j=1}^q m_j = n$. The subspace of eigenvectors associated to the eigenvalue λ_j ,

$$E_{\lambda_j} = \{\mathbf{y} \in \mathbb{C}^n : A\mathbf{y} = \lambda_j\mathbf{y}\},$$

is such that its dimension is less than or equal to the algebraic multiplicity of λ_j . That is, $\dim \ker(A - \lambda_j I) \leq m_j$.

Generalized eigenvectors are vectors such that

$$(A - \lambda I)^k \mathbf{y} = 0, \quad (A - \lambda I)^{k-1} \mathbf{y} \neq 0 \quad (2.1)$$

for some $k > 0$. The vector in (2.1) would be called a k th order, or rank k , generalized eigenvector. An eigenvector is a generalized eigenvector of rank 1.

Given an eigenvalue λ and a generalized eigenvector $\mathbf{v}_k$ of rank k , define the set of vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ by

$$\mathbf{v}_{k-j} = (A - \lambda I)^j \mathbf{v}_k, \quad j = 1, 2, \dots, k - 1.$$

This set is called a chain of generalized eigenvectors (of length k). Then, the vector $\mathbf{v}_j$ is a generalized eigenvector of rank j . One very useful fact about chains of generalized eigenvectors is that they are linearly independent sets. Moreover, if an eigenvalue λ has algebraic multiplicity m , then there exist ℓ chains of generalized eigenvectors, each of length k_q , such that $\sum_{1 \leq q \leq \ell} k_q = m$ and such that the set of all these chains is a linearly independent set.

2.1.1 Dynamical systems of ODEs

Models of mechanical systems are often formulated in the language of linear algebra. The essential ingredients in these systems are – in particular – masses and forces.

One pioneer in the research field of mechanics (and in many others, such as microscopy) was Robert Hooke [65]. Hooke wrote “ut tensio, sic vis” in 1678, meaning that the force of a spring is proportional to its extension, see Figure 2.1. By Newton’s laws, this would mean that a weight that is suspended on a spring is accelerated at a rate proportional to the displacement. Notice that the force is in the opposite direction to the extension, that is, if x is the extension, then $-kx$ is the force. Here $k > 0$ is the proportionality constant.

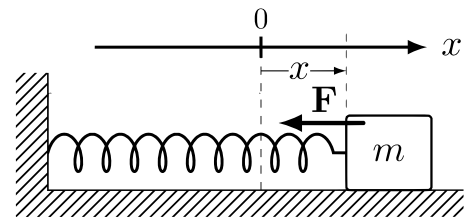


Figure 2.1: The force F of a spring is proportional to its extension x .

The dynamics of the weight-on-a-spring system is described by its position and its velocity. The information given by x at time t reveals the state of the system at this time; the available values of positions and velocities are the possible *configurations* of the system. The time derivative of the position, the velocity dx/dt , is denoted by $\dot{x}$, and the acceleration is $d^2x/dt^2 = \ddot{x}$. Newton’s law of motion ($F = m\mathbf{a}$) and Hooke’s law conclude that the

motion of the weight is described by $m\ddot{x} = -kx$. Introduce the notation $a = k/m$ and let x_1 be the position, while the velocity is denoted by x_2 . This leads to the equations

$$\begin{aligned}\dot{x}_1 &= x_2 \\ \dot{x}_2 &= -ax_1.\end{aligned}$$

The linear algebra formulation is given in terms of the matrix A and the vector $\mathbf{x}$ whose components are x_1 and x_2 . The dot over $\mathbf{x}$ is the time derivative applied to each component:

$$\dot{\mathbf{x}} = A\mathbf{x}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad A = \begin{bmatrix} 0 & 1 \\ -a & 0 \end{bmatrix}.$$

Consider the spring and weight from the above example, this time with an additional damping force, which is proportional to the velocity (that is, a viscosity). The equations will be

$$\begin{aligned}\dot{y}_1 &= y_2 && \text{(velocity)} \\ \dot{y}_2 &= -by_2 - ay_1 && \text{(acceleration)}\end{aligned}$$

It is assumed that $a, b > 0$. This system is equal to $\dot{\mathbf{y}} = A\mathbf{y}$ for

$$A = \begin{bmatrix} 0 & 1 \\ -a & -b \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

The characteristic polynomial of A is in this case $\det(A - \lambda I) = \lambda^2 + b\lambda + a$. In case the damping b is equal to $2\sqrt{a}$, the polynomial has only one real root with algebraic multiplicity 2, namely $\lambda = -\sqrt{a}$. The associated eigenvector is

$$\mathbf{v}_1 = \begin{bmatrix} -1/\sqrt{a} \\ 1 \end{bmatrix}.$$

One solution to the system $\dot{\mathbf{y}} = A\mathbf{y}$ is therefore $\mathbf{y}(t) = \mathbf{v}_1 e^{-\sqrt{a}t}$, since then the time derivative is $\dot{\mathbf{y}}(t) = -\sqrt{a}\mathbf{v}_1 e^{-\sqrt{a}t} = A\mathbf{v}_1 e^{-\sqrt{a}t}$. Solving $\mathbf{v}_1 = (A - \lambda I)\mathbf{v}_2$, a generalized eigenvector is obtained:

$$\mathbf{v}_2 = \begin{bmatrix} -1/a \\ 0 \end{bmatrix}.$$

It can be verified by direct computation that another solution to the system $\dot{\mathbf{y}} = A\mathbf{y}$ is

$$\mathbf{y}(t) = t\mathbf{v}_1 e^{-\sqrt{a}t} + \mathbf{v}_2 e^{-\sqrt{a}t}.$$

There are now two solutions to the dynamical system, and if there are initial conditions on the position and the velocity, that is on y_1 and y_2 , then it is necessary to include both solutions in the general solution. A linear combination of the solutions is

$$\mathbf{y}(t) = a_1 \mathbf{v}_1 e^{-\sqrt{a}t} + a_2 (t\mathbf{v}_1 + \mathbf{v}_2) e^{-\sqrt{a}t}$$

for two constants a_1 and a_2 . At initial time, which is assumed to be $t = 0$ for convenience,

$$\mathbf{y}(0) = a_1 \mathbf{v}_1 + a_2 \mathbf{v}_2 = a_1 \begin{bmatrix} -1/\sqrt{a} \\ 1 \end{bmatrix} + a_2 \begin{bmatrix} -1/a \\ 0 \end{bmatrix}.$$

The velocity condition at $t = 0$ will determine a_1 , since the second component of $\mathbf{v}_2$ is zero, and then the position at $t = 0$ determines a_2 .

In general, if $\mathbf{v}_1, \dots, \mathbf{v}_k$ is a chain of generalized eigenvectors to the matrix A , the following are solutions to $\dot{\mathbf{y}} = A\mathbf{y}$ and they are linearly independent:

$$\begin{aligned} \mathbf{y}_1(t) &= \mathbf{v}_1 e^{\lambda t} \\ \mathbf{y}_2(t) &= (t\mathbf{v}_1 + \mathbf{v}_2) e^{\lambda t} \\ &\vdots \\ \mathbf{y}_k(t) &= \left(\frac{t^{k-1}}{(k-1)!} \mathbf{v}_1 + \dots + \frac{t^2}{2} \mathbf{v}_{k-2} + t\mathbf{v}_{k-1} + \mathbf{v}_k \right) e^{\lambda t} \end{aligned}$$

A linear combination of these is a solution by the principle of superposition. There is a very convenient way to write the general solution of a system of linear ODEs with constant coefficients given initial conditions. The matrix exponential $U(t) = e^{tA}$ of $A \in \mathbb{C}^{n \times n}$ is defined by

$$e^{tA} = \sum_{k=0}^{\infty} \frac{t^k}{k!} A^k = I + tA + \frac{t^2}{2} A^2 + \frac{t^3}{6} A^3 + \dots \quad (2.2)$$

where I is the identity matrix of size $n \times n$. The series in (2.2) converges for any matrix A and t . The matrix exponential e^{tA} is invertible for all t and $(e^{tA})^{-1} = e^{-tA}$, and if A is real-valued then e^{tA} is real-valued for all t .

Theorem: The solution to $\dot{\mathbf{y}} = A\mathbf{y}$ with $\mathbf{y}(0) = \mathbf{y}_0$ is $\mathbf{y}(t) = e^{tA}\mathbf{y}_0$.

In order to fully understand the matrix exponential and the properties of the solution in this theorem, the next section introduces the *Jordan canonical form* of the matrix A .

2.1.2 The Jordan canonical form

Every $n \times n$ matrix A has a Jordan decomposition, $A = QJQ^{-1}$, where Q is an invertible matrix and J is a block diagonal matrix. The columns of Q are generalized eigenvectors. Each block in J is a so-called Jordan block. If $j \geq 1$, define the Jordan block $J_j(\lambda)$ to be the $j \times j$ matrix with λ s on the main diagonal, 1s above the diagonal, and 0s elsewhere. That is,

$$J_1(\lambda) = [\lambda], \quad J_2(\lambda) = \begin{bmatrix} \lambda & 1 \\ 0 & \lambda \end{bmatrix}, \quad J_3(\lambda) = \begin{bmatrix} \lambda & 1 & 0 \\ 0 & \lambda & 1 \\ 0 & 0 & \lambda \end{bmatrix}, \quad \dots \quad (2.3)$$

Putting the 1's above the diagonal is a choice by convention, and it is equally good to define these block matrices with 1's below the diagonal. The Jordan decomposition is unique up to reordering of the blocks and the vectors in Q .

The matrix A is diagonalizable when every Jordan block of A is 1×1 . In that case, the characteristic polynomial of A is a product of distinct factors $(\lambda - \lambda_j)$, that is, in

$$\det(A - \lambda I) = (\lambda_1 - \lambda)^{m_1} (\lambda_2 - \lambda)^{m_2} \cdot \dots \cdot (\lambda_q - \lambda)^{m_q}$$

all m_j would equal 1 and $q = n$. The algebraic multiplicity and the geometric multiplicity reveals some of the key information about the Jordan form J .

- The algebraic multiplicity of λ_j is the number of λ_j 's along the diagonal of J .
- The geometric multiplicity of λ_j is the number of Jordan blocks with eigenvalue λ_j .

In order to completely determine the Jordan form of a matrix, define the “deficiency indices” $\delta_\ell = \dim \ker(A - \lambda I)^\ell$. Let r be the smallest integer for which $(A - \lambda I)^r = (A - \lambda I)^{r+1}$. Then compute δ_ℓ for $\ell = 1, 2, \dots, r$. The number of Jordan blocks of size ℓ is given by [64]

$$\begin{aligned} v_1 &= 2\delta_1 - \delta_2, & v_r &= \delta_r - \delta_{r-1} \\ v_j &= 2\delta_j - \delta_{j+1} - \delta_{j-1} & \text{for } j &= 2, 3, \dots, r-1. \end{aligned}$$

If A is a real matrix, then the characteristic polynomial has real coefficients and any complex eigenvalue would therefore occur together with its complex conjugate. In the above Jordan form, if $\alpha + i\beta$ occurs on the diagonal, there would also be just as many $\alpha - i\beta$ on the diagonal. The matrices

$$\begin{bmatrix} \alpha & \beta \\ -\beta & \alpha \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \alpha + i\beta & 0 \\ 0 & \alpha - i\beta \end{bmatrix} \quad (2.4)$$

are similar via the transformation,

$$\begin{bmatrix} \alpha & \beta \\ -\beta & \alpha \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \begin{bmatrix} \alpha + i\beta & 0 \\ 0 & \alpha - i\beta \end{bmatrix} \begin{bmatrix} 1 & -i \\ 1 & i \end{bmatrix}. \quad (2.5)$$

Therefore, if A is a real matrix, it admits a real Jordan form, which instead of having eigenvalues $\alpha \pm i\beta$ on the diagonal and 1s above has

$$\begin{bmatrix} \alpha & \beta \\ -\beta & \alpha \end{bmatrix} \quad (2.6)$$

on the diagonal and 2×2 identity matrices above those blocks [64]. Assume that A is $2k \times 2k$ and has precisely $2k$ distinct eigenvalues $\lambda_j = \alpha_j + i\beta_j$ and $\bar{\lambda}_j = \alpha_j - i\beta_j$ with complex generalized eigenvectors $\mathbf{w}_j = \mathbf{u}_j + i\mathbf{v}_j$ and $\bar{\mathbf{w}}_j = \mathbf{u}_j - i\mathbf{v}_j$ for $j = 1, 2, \dots, k$. Here, $\mathbf{u}_j$ and $\mathbf{v}_j$ are the real and imaginary parts of $\mathbf{w}_j$. Then the square matrix with columns

$$P = \begin{pmatrix} \mathbf{u}_1 & \mathbf{v}_1 & \mathbf{u}_2 & \mathbf{v}_2 & \dots & \mathbf{u}_k & \mathbf{v}_k \end{pmatrix} \quad (2.7)$$

is invertible and

$$P^{-1}AP = \text{diag}(R_j), \quad \text{with } R_j = \begin{bmatrix} \cos \beta_j t & \sin \beta_j t \\ -\sin \beta_j t & \cos \beta_j t \end{bmatrix}.$$

This yields the *real* Jordan form of A . Every square, real matrix has a real Jordan form.

2.1.3 The fundamental solution to the Cauchy problem

Let A be a real $n \times n$ matrix and let $\mathbf{y}_0$ be a given, fixed vector in $\mathbb{R}^n$ and consider the initial value problem

$$\dot{\mathbf{y}} = A\mathbf{y}, \quad \mathbf{y}(0) = \mathbf{y}_0. \quad (2.8)$$

This is called a Cauchy problem, after Cauchy who correctly stated the conditions needed for such problems to have a well-defined solution [30].

Consider a real eigenvalue λ and a $k \times k$ Jordan block matrix J with all λ on the diagonal, that is,

$$J = \begin{bmatrix} \lambda & 1 & 0 & \dots & 0 \\ 0 & \lambda & 1 & \dots & 0 \\ 0 & 0 & \lambda & \dots & 0 \\ \vdots & & & \ddots & \\ 0 & 0 & 0 & \dots & \lambda \end{bmatrix}.$$

Decomposing this into $J = D + N$, where D is the diagonal part of J and N is the 1s on the diagonal above the main diagonal. Then, N is nilpotent [26] of order k (that is, N^{k-1} is not the zero matrix, but N^k is the zero matrix). Moreover,

$$e^{tJ} = e^{\lambda t} e^{tN} = e^{\lambda t} \begin{bmatrix} 1 & t & \frac{t^2}{2} & \dots & \frac{t^{k-1}}{(k-1)!} \\ 0 & 1 & t & \dots & \frac{t^{k-2}}{(k-2)!} \\ 0 & 0 & 1 & \dots & \frac{t^{k-3}}{(k-3)!} \\ \vdots & & & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}. \quad (2.9)$$

Recall that A is assumed to be a real, square matrix, and the complex eigenvalues therefore occur in pairs of complex conjugates. If there is an eigenvalue pair $\alpha \pm i\beta$ then this pair produces the Jordan block

$$e^{tJ} = e^{\alpha t} \begin{bmatrix} R & tR & \frac{t^2}{2}R & \dots & \frac{t^{k-1}}{(k-1)!}R \\ 0 & R & tR & \dots & \frac{t^{k-2}}{(k-2)!}R \\ 0 & 0 & R & \dots & \frac{t^{k-3}}{(k-3)!}R \\ \vdots & & & \ddots & \vdots \\ 0 & 0 & 0 & \dots & R \end{bmatrix}, \quad (2.10)$$

where R is the “rotation” 2×2 matrix

$$\begin{bmatrix} \cos \beta t & \sin \beta t \\ -\sin \beta t & \cos \beta t \end{bmatrix}.$$

These are the forms of the Jordan blocks that are produced by the real matrix A . The number of blocks are determined by the multiplicities and deficiency indices for each eigenvalue. To each eigenvalue, there is a sequence of generalized eigenvectors, as explained in §2.1.1. In order to write down the solution to the problem (2.8), let $2n - k$ be the size of the matrices, that is, assume that A is $(2n - k) \times (2n - k)$. If there are k real eigenvalues λ_j for $j = 1, 2, \dots, k$, and complex eigenvalues $\lambda_j = \alpha_j + i\beta_j$, $\bar{\lambda}_j = \alpha_j - i\beta_j$, for $j = k + 1, \dots, n$, then there exists a basis of $\mathbb{R}^{2n-k}$, namely

$$\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k, \mathbf{u}_{k+1}, \mathbf{v}_{k+1}, \dots, \mathbf{u}_n, \mathbf{v}_n\}. \quad (2.11)$$

Here $\mathbf{u}_1, \dots, \mathbf{u}_k$ correspond to λ_j , $j = 1, \dots, k$ while the complex eigenvalues $\alpha_j \pm i\beta_j$ have eigenvectors $\mathbf{u}_{k+1} \pm i\mathbf{v}_{k+1}, \dots, \mathbf{u}_n \pm i\mathbf{v}_n$. Let P be the square matrix with the columns of (2.11). Then, the solution to the above Cauchy problem is

$$\mathbf{y}(t) = P \operatorname{diag}(e^{tJ_k}) P^{-1} \mathbf{y}_0,$$

where J_k are the Jordan blocks [64]. This implies that each component of the solution $\mathbf{y}(t)$ is a linear combination of either

$$t^l e^{\alpha_j t} \cos(\beta_j t) \quad \text{or} \quad t^l e^{\alpha_j t} \sin(\beta_j t)$$

where $0 \leq l \leq k - 1$ and $\lambda_j = \alpha_j + i\beta_j$ produces a $k \times k$ block of type (2.9) if $\beta_j = 0$ or, otherwise, a $2k \times 2k$ block of type (2.10). If $k = 1$ in all these blocks, there are no polynomials t^l in the components and A is called semi-simple. That is, A is called semi-simple if the Jordan form of A contains only diagonal 1's or R 's. Assuming A is semi-simple and that its eigenvalues have non-positive real parts, the Cauchy problem (2.8) has a bounded solution for all $t > 0$. On the other hand, even if the eigenvalues of A have non-positive real parts, if A is not semi-simple then there exists a $\mathbf{y}_0$ such that $|\mathbf{y}(t)| \rightarrow \infty$ as $t \rightarrow \infty$.

2.2 Foundations of non-cooperative games

Game theory is the study of decision-making in a context with specific rules. Decisions are made by *players* and these players have a notion of *payoff* such that the rational choices from each player's perspective are increasing the payoff. Oftentimes, the rational choice from a player's perspective is not constituting the best collective action; what benefits everyone the most is perhaps not achieved because it does not seem rational from an individual perspective. These insights are highlighted by game theory thanks to its simple rules.

One of the situations that were formalized in the founding work *Theory of Games and Economic Behaviour* [76] was a 2-player game that is such that one player's win is the other's loss, in other words, the payoff to either player is the negative of the payoff to the other: If player *A* receives p then player *B* receives $-p$. For this reason, the game is called *zero-sum*, as the payoffs sum up to zero. More generally, some games are "constant sum games" if the payoffs are adding up to the same number, or, say, 100%.

There are two formulations for two-person zero-sum games with a finite number of alternatives for each player: the normal form and the extensive tree form [32]. The normal form is also called strategic form [53]. The payoffs can be arranged in a matrix in some games, giving the matrix form games, and §2.2.1 will contain an example of this based on climate agreements. The payoffs in normal form games are determined only on the basis of the strategies that each player chooses "here and now". In tree form games, on the contrary, the players' strategies and payoffs can be determined or influenced in a time sequence and the choices of strategies can depend on the previous events [53]. Only the normal form games are considered in this thesis. Then, a payoff is a mapping that outputs a real number based on all the players' strategies. The set of possible strategies may possess almost any structure, such as a finite set of values, a subset of $\mathbb{R}^n$, a set of measurable functions, etc.

We continue this chapter with one of the most important results of game theory, namely an explanation of *the tragedy of the commons*. In a group

of decision-makers, the tragedy of the commons is in general a situation where no participant seeks to cooperate for the common good even though such cooperation would benefit every participant.

2.2.1 A motivating example in game theory

Climate change is a major issue that requires negotiation between countries. Consider a meeting between two countries that can either defect from an issued agreement or decide to cooperate within the agreement. If both cooperate, they each get a climate benefit of 6 (in some unit, e.g. a monetary currency or natural resources), whereas if only one of them cooperates they receive a lower climate benefit of 3. Cooperating requires the country to take action to mitigate further global warming, and that costs 4. That is, if both cooperate, both get $6 - 4 = 2$. If both defect, both get $0 - 0 = 0$. If one cooperate and the other defects, the cooperator gets $3 - 4 = -1$, and the defector gets $3 - 0 = 3$. Here is a table summarizing these payoffs:

Player A's strategy	Cooperate	Cooperate	Defect	Defect
Player B's strategy	Cooperate	Defect	Cooperate	Defect
Player A's payoff	2	-1	3	0
Player B's payoff	2	3	-1	0

Now each country has the following options to consider: If the other country decides to cooperate, then defecting guarantees a benefit of 3 while cooperating gives 2. If the other country decides to defect, then defecting comes with a benefit of 0 and cooperating gives -1 . That is, if the other's strategy is not known then it is better to defect. Both players will therefore defect as they do not trust the other player to cooperate even though the common good would benefit most if both would cooperate. This situation is the essential mechanism of the tragedy of the commons.

A. Tucker named the above game the *prisoners' dilemma* (PD) to popularize game theory to the psychology community. M. Flood and M. Dresher discussed games with the structure of prisoner's dilemma in 1950, and so did also Nash, but none of them published their ideas immediately [46].

It is standard procedure to write these possible outcomes in a matrix as in the figure below. Here, C denotes the option “cooperate” and D denotes “defect”. Each box contains the gain to each player such that the top-right number belongs to the player B and the bottom-left number goes to player A . This example is symmetric since both players have the same set of actions and are paid the same payoffs.

		player B	
		C	D
player A	C	2 2	-1 3
	D	3 -1	0 0

Symmetric games are those games where every player can choose from the same set of actions and the payoffs depend only on all the strategies employed, not on which player is playing them. In a symmetric game, the game payoffs can be represented by the matrix

$$M = \begin{bmatrix} R & S \\ T & P \end{bmatrix}. \quad (2.12)$$

The entries are the payoffs to player A , where the top row is the payoff if A plays “cooperate” and the bottom row correspond to A playing “defect”. The payoff matrix for the other player is the transpose matrix. In the above case, $R = 2$, $S = -1$, $T = 3$ and $P = 0$. Now we can define what the prisoner’s dilemma is mathematically: It is the situation

$$T > R > P > S. \quad (2.13)$$

2.2.2 Strategies and Nash’s concept of equilibrium

A distribution of probabilities over the set of possible actions is called a *mixed strategy*. In the example above there were two options (C and D) for each player, so if a player plays C with probability x then the same player

chooses D with probability $1 - x$. In this case we can compute what payoff is *expected*. The payoff which A expects when A plays the mixed strategy $\mathbf{x} = (x, 1 - x)$ and B plays $\mathbf{y} = (y, 1 - y)$ is then $p_y(\mathbf{x}) = \mathbf{x} \cdot M\mathbf{y}$, where M is the matrix (2.12). A *pure strategy* assigns probability 1 to only one option. In the prisoner's dilemma, pure strategies correspond to choosing either cooperate or defect with full certainty.

In *non-cooperative* game theory, players do not reveal their intentions to other players and they therefore act only to maximize the individual payoff that they receive. In contrast to this, cooperative games follow a different set of rules. There are no individual payoffs but the game has an overall value which is determined by the values of the “coalitions” that form in the game. This thesis will only concern non-cooperative games, but the interested reader is encouraged to consult the founding works by Shapley [72] for an introduction to cooperative games.

In this thesis we consider repeated games with the possibility to change action when a new turn is played as long as there is a fixed probability distribution of choices. It is assumed that history is irrelevant in the sense that the game stays in normal form, that is, the strategies are not dependent on previous events.

The concept of rational decision from an individual's point of view is captured mathematically by the notion of *equilibrium*. In an equilibrium, no player has incentive to change strategy. Borel formulated and studied game equilibria in the early 20th century for two-player games and same did von Neumann during the 20's though the 40's. The equilibrium concept was extended to include n players by J. Nash in the 50's. [32] Nash proved that any game with n players has a symmetric equilibrium [58] and a game's equilibrium is therefore often called *Nash equilibrium*. In the above example, there is an equilibrium when both players defect. Mathematically, an equilibrium is defined as a set of strategies such that no player has incentive to change strategy, assuming the other players' strategies are unchanged. If we let $\{f_i\}_{i=1}^n$ denote a set of strategies and p_i denotes the payoff to player i , then $\{f_i\}_{i=1}^n$ is an equilibrium if for every i

$$p_i(f_1, \dots, f_n) = \max_{g_i \in S} p_i(f_1, \dots, f_{i-1}, g_i, f_{i+1}, \dots, f_n). \quad (2.14)$$

Here, S is the set of possible strategies. The strategies in an equilibrium are called equilibrium strategies or sometimes just *optimal* [53]. As an example, an equilibrium in a 2-player game is a pair of strategies (f_1, f_2) meeting the conditions

$$\begin{aligned} p_1(f_1, f_2) &\geq p_1(g_1, f_2) \\ p_2(f_1, f_2) &\geq p_2(f_1, g_2) \end{aligned}$$

for arbitrary strategies g_1 and g_2 . If the game is zero-sum, then $p_1(f_1, f_2) + p_2(f_1, f_2) = 0$.

In Chapter 3, the above symmetric matrix game plays a particularly important role in the context of changing behaviors during a disease outbreak. Chapter 4 of this thesis investigates the Nash equilibria of a game of competing teams.

2.2.3 A motivating example in population dynamics

In 1973, almost thirty years after the publication of von Neumann and Morgenstern's founding work, Maynard Smith and Price [52] asked: "How can one explain such oddities as snakes that wrestle with each other, deer that refuse to strike 'foul blows', and antelope that kneel down to fight?" They used game theory and their newly developed notion of *evolutionarily stable strategies* (ESS) to explain why fighting between members of the same species usually do not escalate unless the opponent aim to cause severe injury. In this context, the strategies "cooperate" and "defect" are termed "conventional conflict" and "dangerous conflict" and the fights are represented by a matrix-game, similar to the prisoner's dilemma. The payoff is interpreted as a Darwinian fitness, that is, a survival advantage.

At an ESS, if a mutant appears then the resident (or "original") population performs better against the mutant than the mutant itself. In equations, this means that there is an additional stability condition apart from the equilibrium condition. Let $p(f, g)$ be the payoff to an individual playing strategy f against another strategy g . Then, f is an ESS if [67]

- (Equilibrium condition.) $p(f, f) \geq p(g, f)$ for all g ,

- (Stability condition.) If g performs equally well against f , then f performs better against g than g against g , that is,

$$p(g, f) = p(f, f) \implies p(f, g) > p(g, g).$$

The importance of an ESS is understood in an ecological context; if the strategies of the players are not rational choices but rather implications of their characteristics, which adhere to the laws of evolution, then the strategies should have the possibility to change in a way similar to the genetic change that mutations introduce in nature. This process can result in strategies that are different from the strategic games from the previous section. The ESS conditions ensure that deviations from the equilibria gain fitness from going back to the equilibrium. We will encounter a version of these ideas in Chapter 3 when we consider games in combination with epidemiological models and identify the stable steady state solutions. In the next section, we specify some of the mathematical models of the laws of evolution from the literature. Moreover, the ESS concept is revisited.

2.2.4 Evolutionary game theory

Recall that a mixed strategy is a probability distribution over the options in a game. Consider a mixed strategy with two options, $x = (x, 1 - x)$, and denote by p_x the payoff for playing “cooperate” when the opponent assumes the strategy x . Assuming that the other player in a 2-player game can choose from the same set of actions, what is a reasonable change of strategy if we start at the mixed strategy x ?

Replicator equations of symmetric games

In most classical applications, game theory focuses on decisions made by rational players using cognitive choice. On the contrary, the evolutionary application of games specifies a process of natural selection—individuals are merely the performers of an inherited program. In a 2-player symmetric game with two options, such as prisoner’s dilemma, a mixed strategy x (meaning that the other option is chosen with probability $1 - x$) could

develop according to a “replicator’s equation”, which is formulated as

$$\dot{x} = F(x) \quad (2.15)$$

and which specifies the change of the strategy. Since the game is symmetric and 2-player, only one payoff function is needed. A common assumption is that the strategy changes in proportion to the payoff’s linear deviation from the mean value of the payoff, that is $F(x) = x(p_x - \langle p \rangle)$, where p_x is the payoff when the strategy x is played by the other player and $\langle p \rangle$ is the mean value of the payoffs. Recall the payoff matrix from §2.2.1. Let $\mathbf{x}$ be the vector with components x and $1 - x$ and let e_1 be the first unit vector:

$$\mathbf{x} = \begin{bmatrix} x \\ 1 - x \end{bmatrix}, \quad e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

Then

$$\frac{d}{dt}x = e_1 \cdot M\mathbf{x} - \mathbf{x} \cdot M\mathbf{x}.$$

The right hand side of this equation is the difference between playing cooperate as a pure strategy and playing cooperate with probability x . Thus, in the symmetric 2×2 matrix-form game we have

$$\begin{aligned} \dot{x} &= x(Rx + S(1 - x) - Rx^2 - Sx(1 - x) - Tx(1 - x) - P(1 - x)^2) \\ &= x(Rx(1 - x) + S(1 - x)^2 - Tx(1 - x) - P(1 - x)^2) \\ &= x(1 - x)(Rx + S(1 - x) - Tx - P(1 - x)) \\ &= -x(1 - x)((T - R)x + (P - S)(1 - x)). \end{aligned} \quad (2.16)$$

We can write $\dot{x} = -x(1 - x)(D_g x + D_r(1 - x))$, where $D_g = T - R$ and $D_r = P - S$. A special case of the PD game is the *Donor-Recipient game* which has $D_g = D_r$, meaning that the payoff advantage of defection over cooperation is independent of the opponent’s choice [75]. Denoting the payoff disadvantage by C (for “cost”) we write $D_g = D_r = C$. In the donor recipient game,

$$\dot{x} = -x(1 - x)C. \quad (2.17)$$

Without loss of generality, one can assume that $P = 0$. In accordance with the PD-condition (2.13) we require

$$-C < 0 < R < R + C \quad (2.18)$$

and the payoff matrix becomes

$$\begin{bmatrix} R & -C \\ R + C & 0 \end{bmatrix}. \quad (2.19)$$

In the next sections, we will formulate the dynamics using R and C only, and forget S , T and P .

Network reciprocity

Networks in games represent contacts between players. The contacts enable the players to interact, so for instance, in the context of disease spreading there are a limited number of possible transmission paths of the disease. We make the following assumptions:

1. What two-steps neighbors do is irrelevant.
2. We assume the graph is degree-regular, meaning that each node has the same number, k , of connecting edges.

Under these assumptions the cost C in the donor recipient game decreases by $N(k)$, where [75, 61]

$$N(k) = \frac{Rk - 2C}{(k + 1)(k - 2)}, \quad k \neq 2, \quad N(2) = R.$$

Notice that $N(k) \rightarrow 0$ if $k \rightarrow \infty$, which reflects the fact that unlimited network connectivity recovers the network-free, well-mixed situation. Now the equation (2.16) modifies by the change of the payoff matrix to

$$\dot{x} = -x(1 - x)(C - N(k)). \quad (2.20)$$

By (2.18), the game is of PD type when $N(k) - C < 0 < R$, which is equivalent to

$$0 < R < C(k - 1). \quad (2.21)$$

That is, the benefit of mutual cooperation compared to the cost of mitigation determines whether the game is of PD type. For example, when R/C is large, corresponding to low costs of mitigation and/or high benefit of

mutual cooperation, the game may cease to be of PD type for values of sufficiently small values of k such that (2.21) breaks. For sufficiently large values of k , in particular for well-mixed populations, the game is always of PD type.

2.2.5 Adaptive dynamics

The concept of ESS is limited to a “static” analysis; it says when an equilibrium enjoys stability, but it does not reveal if the ESS are established by any dynamics over time. In order to use game theory as a model for natural evolution, it is interesting to construct a game theoretical natural selection process. This motivated the field of adaptive dynamics, which considers the evolution of game strategies and whether the dynamics of the game at hand can establish the equilibrium strategies. Several scenarios are possible in a population which experiences evolution through the process of mutations: the new mutations can lead to a complete trait exchange of the population, or the population remains as is (that is, the mutation goes extinct), or the species diverges into separate species, and so on. The analysis by Geritz *et al.* [25] starts at the following assumptions:

- Individuals replicate, that is, their offspring is identical to the parent.
- The success of a mutation can be inferred from its growth rate inside the resident population while the mutation is still very rare.
- Mutations are small but random.

The analysis proceeds via the assumption that a population is in a stationary state before the (rare) mutation appears, and it is further assumed that the result of this mutation is known before the occurrence of any new mutations. This reflects a kind of scale-separation on the evolutionary time axis [45]. The initial growth rate of a mutant is called the invasion fitness. If the species can be characterized by a scalar-valued trait, let x be the resident population’s trait and denote by $s_x(y)$ the invasion fitness of a mutant having trait y . If $s_x(y) > 0$, the mutant experiences growth but if $s_x(y) < 0$ it will go extinct. The invasion fitness is usually represented in a so-called pairwise invasibility plot, which displays the sign of $s_x(y)$ as a

function of both x and y . Since the resident population is assumed to be in a stationary state, the line $x = y$ shows $s_x(x) = 0$. Referring to Figure 2.2, the black lines show the zero level set of $s_x(y)$. Whenever a line crosses the diagonal, there is an evolutionarily singular strategy, x^* . If $s_{x^*}(y) < 0$ for all y except x^* in a neighborhood around x^* , the singular strategy is locally ESS-stable in the sense of Maynard Smith [51]. This leads to the criterion

$$\frac{\partial^2 s_x(y)}{\partial y^2} < 0$$

on the invasion fitness at $x = y = x^*$ for it to be ESS stable. Another stability criterion is the *convergence stability* of a singular strategy x^* . It is defined in a neighborhood around x^* such that if $x < y < x^*$ or $x^* < y < x$ then $s_x(y) > 0$, which means that a strategy close to a singular strategy would be invaded by mutants that approach the singular strategy. If $s_x(y)$ is at least twice differentiable, convergence stability is characterized by

$$0 < \frac{\partial^2 s_x(y)}{\partial x^2} - \frac{\partial^2 s_x(y)}{\partial y^2}.$$

Convergence stability and ESS stability are independent criteria in the sense that there are singular strategies that are stable in either way but not the other, and they could be both ESS stable and convergence stable. In an initially monomorphic population, singular strategies that are convergence stable but not ESS stable are evolutionary attractors, but as soon as the singular strategy is established, the population tends to diverge. It is a branching point [25].

Dieckmann et al. [15] proposed a framework for adaptive dynamics on function-valued traits based on approximations to stochastic models, assuming that (a) mutations make small changes to the traits, and that (b) the natural selection occurs much faster than the typical time between the appearance of novel mutations, so that each population is monomorphic. The functions that represent traits belong to a trait space (a function space) which is selected based on modeling principles. They consider functions of a single, real variable.

The result of these considerations is that a trait function f develops ac-

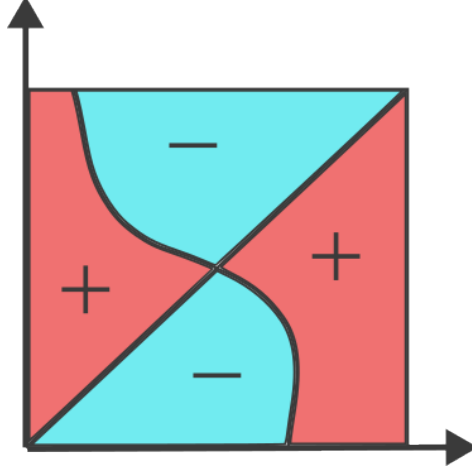


Figure 2.2: A pairwise invasibility plot.

cording to the differential equation

$$\frac{d}{dt}f(x) = \frac{1}{2}\mu_f\bar{n}_f \int_{\Omega} \sigma_f^2(x, y)g_f(y) dy, \quad (2.22)$$

which is called the canonical equation of function-valued adaptive dynamics. It applies to rare mutations that make small and symmetric changes to the function traits. Here, μ_f is the probability distribution of mutations around the trait f , and $\bar{n}_f$ denotes the equilibrium population size of the resident population. The variance-covariance function σ_f^2 captures cross-dependences if changes at $f(y)$ influence the change at $f(x)$. The domain of integration, Ω , is selected based on the model. The function g_f is the selection gradient

$$g_f(x) = \left. \frac{d}{dt} \right|_{t=0} s_f(f + t\delta_x),$$

where $s_f(h)$ is the invasion fitness of h in the resident population f and δ_x is the Dirac delta centered at x . The stability modes (ESS stability, convergence stability, etc.) can now be characterized for the Hessian matrix of $s_f(h)$ by taking functional derivatives with respect to f and/or h . For details, see Dieckmann *et al.* [15].

2.3 Analysis: Banach spaces, integration

One of the standard examples of a Banach space is the space of continuous functions on the unit interval $[0, 1]$. The Euclidean space $\mathbb{R}^n$ of n -dimensional vectors with the inner product

$$\langle x, y \rangle = \sum_{i=1}^n x_i y_i$$

is also a Banach space. More generally, a Banach space is a normed, complete vector space. A vector space V is said to be normed if any point x in V can be associated to a non-negative number $\|x\|$ called the norm of x via a norm function $\|\cdot\|$ such that

1. $\|x + y\| \leq \|x\| + \|y\|$ for all $x, y \in V$,
2. $\|ax\| = |a|\|x\|$ if $x \in V$ and a is a scalar, and
3. $\|x\| > 0$ whenever $x \neq 0$.

A norm induces a distance, or metric, between points in the vector space via $\rho(x, y) = \|x - y\|$. Given a metric ρ on V , the open ball with radius r centered at x is the set $B_r(x) = \{y \in V : \rho(x, y) < r\}$. A topological space is a set with a definition of open sets in the set, for example normed vector spaces, since a distance function provides a natural topology to a vector space [71].

A linear map from a set V into (possibly another set) U is a mapping $A : V \rightarrow U$ such that $A(ax + by) = aA(x) + bA(y)$ for all $x, y \in V$ and all scalars a and b . Linear maps of V into the scalars of V are called linear functionals. Given two normed vector spaces (or more generally two topological vector spaces) V and U and a linear map $A : V \rightarrow U$, this map is said to be bounded if it maps bounded sets into bounded sets. In other words, A is bounded means that $A(E)$ is a bounded subset of U for every bounded set E in V . The space of bounded linear mappings on V can be given the structure of a vector space under the addition operation and multiplication by scalars. A special case is the bounded linear mappings from V into the scalars, denoted by V^* and which is usually called the dual space of V .

If V and U are normed spaces and A is a bounded, linear mapping $V \rightarrow U$, the operator norm can be defined by $\|A\| = \sup\{\|Av\| : v \in V, \|v\| \leq 1\}$. Then the space of bounded linear mappings from V into U is a normed space, and it is a Banach space if also U is a Banach space.

2.3.1 Measurable functions

Let $(X, \mathcal{M})$ and $(Y, \mathcal{N})$ be measurable spaces and let $f : X \rightarrow Y$ be a function. Define the set $f^{-1}(E) = \{x \in X : f(x) \in E\}$. The function f is said to be $(\mathcal{M}, \mathcal{N})$ measurable if $f^{-1}(E) \in \mathcal{M}$ for every $E \in \mathcal{N}$. In particular, f is called Lebesgue measurable when $f : \mathbb{R} \rightarrow \mathbb{C}$ and $\mathcal{N} = \mathcal{B}_{\mathbb{C}}$ is the Borel σ -algebra and $\mathcal{M}$ is σ -algebra of Lebesgue measurable sets.

A so-called simple function on a set E is a measurable function that takes only finitely many (real) values. It is usually written as a sum over its level sets. Let a_i with $i = 1, 2, \dots, n$ be the values that a simple function ψ takes on E . Then $\psi^{-1}(a_i) = E_i$ are the level sets, and

$$\psi = \sum_{i=1}^n a_i \chi_{E_i}.$$

Here, χ_U is defined as the indicator function: $\chi_U(x) = 1$ whenever $x \in U$ and if x is not in U then $\chi_U(x) = 0$. The integral of ψ is defined as

$$\int_E \psi = \sum_{i=1}^n a_i \mu(E_i),$$

where μ is the Lebesgue measure. If f is a bounded, real-valued function defined on a set E of finite measure, define the lower and upper Lebesgue integral of f over E to be

$$\sup \left\{ \int_E \psi : \psi \text{ is simple and } \psi \leq f \text{ on } E \right\},$$

and

$$\inf \left\{ \int_E \psi : \psi \text{ is simple and } \psi \geq f \text{ on } E \right\}.$$

If the lower and upper Lebesgue integral coincide, their value is the *Lebesgue integral* of the function f over E , and f is said to be integrable.

Whenever f is a bounded function on a closed, bounded interval on the form $[a, b]$, then f is Riemann integrable over $[a, b]$ and it is also Lebesgue integrable over $[a, b]$. Moreover, the two integrals are equal [70]. The integral is in this case denoted in the usual way by $\int_a^b f dx$, where dx is the Lebesgue measure. Also, if f is a bounded, measurable function on a set of finite measure E , then f is integrable over E . If f is not defined on a set of finite measure, one approximates f with functions which are defined on sets of finite measures. In that case, f is called integrable if the Lebesgue integral of f is finite.

The *Lebesgue dominated convergence theorem* states that a pointwise convergence can be moved inside an integral under the following conditions: Assume that $\{f_n\}$ is a sequence of measurable functions on E and that there exists an integrable function g on E such that $|f_n| \leq g$ on E for all n . If $f_n \rightarrow f$ pointwise almost everywhere on E , then f is integrable on E and

$$\lim_{n \rightarrow \infty} \int_E f_n = \int_E f.$$

A consequence of the Lebesgue dominated convergence theorem is the following condition for differentiating under the integral. Let $f(x, t)$ be defined on the square domain $\Omega = \{(x, t) : 0 \leq x \leq 1, 0 \leq t \leq 1\}$ and assume that it is a measurable function of x for each fixed value of t . Assume that $\partial f / \partial t$ exists and that there is a function $g \in L^1[0, 1]$ such that

$$\left| \frac{\partial f}{\partial t}(x, t) \right| \leq g(x) \quad \text{on } \Omega.$$

Then

$$\frac{d}{dt} \int_0^1 f(x, t) dx = \int_0^1 \frac{\partial f}{\partial t}(x, t) dx.$$

The existence of $\partial f / \partial t$ can be ensured if $f(x, \cdot)$ is absolutely continuous [23]. Moreover, if $\partial f / \partial t$ is continuous as a function of t for each fixed x , then $F(t) = \int_0^1 f(x, t) dx$ is continuous.

2.3.2 The L^p spaces

Now fix a measure space $(X, \mathcal{M}, \mu)$. Let f be an integrable function on X and define, for p in the range $1 \leq p < \infty$,

$$\|f\|_p = \left(\int_X |f(x)|^p d\mu \right)^{1/p}. \quad (2.23)$$

We define the L^p functions on X to be the set of integrable functions on X for which $\|f\|_p$ is finite, and upon identifying $f = g$ whenever $f = g$ almost everywhere. The norm (2.23) makes $L^p(X)$ into a normed vector space. The norm for $p = \infty$ is

$$\|f\|_\infty = \inf \{C \geq 0 : |f(x)| \leq C \text{ for almost every } x\}.$$

For every $p \geq 1$, these L^p spaces of functions are Banach spaces [23].

The following is the Hölder inequality: For any p in the range $1 < p < \infty$, define p' by $1/p + 1/p' = 1$. If f and g are measurable functions on X , then

$$\|fg\|_1 \leq \|f\|_p \|g\|_{p'}.$$

In particular, if $f \in L^p(X)$ and $g \in L^{p'}(X)$, then $fg \in L^1(X)$. Hölder's inequality holds with equality if and only if $a|f|^p = b|g|^{p'}$ for non-zero constants a and b . The result $\|fg\|_1 \leq \|f\|_p \|g\|_{p'}$ can be extended to $p = \infty$ with $p' = 1$.

The inclusion $0 < p < q \leq \infty \implies L^p[0, 1] \supset L^q[0, 1]$ holds on $[0, 1]$ and on any set of finite measure. For instance, if f has support on the (finite) interval I , by taking the indicator function on I , χ_I , the Hölder inequality gives $\|f\|_1 = \|f\chi_I\|_1 \leq \|f\|_2 \|\chi_I\|_2$, meaning that if $f \in L^2[0, 1]$ then $f \in L^1[0, 1]$. Similarly, $\|f\|_2 \leq C\|f\|_\infty$, for some $C > 0$, on finite sets. The converse is not true. For instance, $f(x) = 1/\sqrt{x}$ is in $L^1[0, 1]$ but $f^2 = 1/x$ is not.

If $1 < p < \infty$ and $1/p + 1/p' = 1$ then for every bounded, linear functional A on $L^p(X)$, there exists $g \in L^{p'}(X)$ such that $A(f)$ is given by the integral against g , that is

$$A(f) = \int_X fg d\mu.$$

Let X and Y be metric spaces with metrics ρ and σ , respectively. A mapping f from X to Y is said to be uniformly continuous if for every $\varepsilon > 0$ there is a $\delta > 0$ such that $\rho(x, x') < \delta$ implies that $\sigma(f(x), f(x')) < \varepsilon$ for all x and x' in X . Let X be the interval $[a, b]$ with possibly $a = -\infty$ and with the Lebesgue measure and the usual metric. Let $f \in L^1[a, b]$ and define F on $[a, b]$ by

$$F(x) = \int_a^x f(y) dy.$$

Then F is uniformly continuous and has finite variation [34]. Conversely, if $-\infty < a < b < \infty$ and F is absolutely continuous then F is differentiable a.e. and $F(x) - F(a) = \int_a^x f(x) dx$ for some $f \in L^1[a, b]$.

Let $(X, \mathcal{M}, \mu)$ and $(Y, \mathcal{N}, \nu)$ be two measure spaces and consider the integral operator $K : L^q(Y) \rightarrow L^p(X)$

$$Kf(x) = \int_Y K(x, y)f(y) d\nu(y).$$

Here, we denote the integral kernel as well as the operator by K . Let $\mathcal{H}_{pq}(X, Y)$ be the set of integral operators K such that

$$k(x) = \|K(x, \cdot)\|_{q'} < \infty$$

for μ -almost all $x \in X$ and $k \in L^p(X)$. Then, for finite p and $q > 1$ the L^p norm of k makes $\mathcal{H}_{pq}(X, Y)$ a Banach space [38]. This norm is the “double norm”

$$\|K\| = \left(\int_X \left(\int_Y |K(x, y)|^{q'} d\nu(y) \right)^{p/q'} d\mu(x) \right)^{1/p}.$$

If $1 \leq p < \infty$ and $1 < q \leq \infty$ then every $K \in \mathcal{H}_{pq}(X, Y)$ is a compact operator $L^q(Y) \rightarrow L^p(X)$. This applies in particular to $\mathcal{H}_{22}(X, Y)$ which are the so-called Hilbert-Schmidt operators [38].

Let $W^{s,p}(U)$ be the Sobolev space of functions on the open subset $U \subset \mathbb{R}^n$ such that their (weak) derivatives of s^{th} order are contained in $L^p(U)$. Here, $p \geq 1$ and s is a positive integer. Let α be a multi-index $\alpha = (\alpha_1, \dots, \alpha_n)$ that defines

$$\partial^\alpha = \frac{\partial^{\alpha_1}}{\partial x^{\alpha_1}} \cdots \frac{\partial^{\alpha_n}}{\partial x^{\alpha_n}}$$

and $|\alpha| = \alpha_1 + \dots + \alpha_n$. The usual norm on $W^{s,p}(U)$ is

$$\|f\| = \sum_{|\alpha| \leq s} \|\partial^\alpha f\|_{L^p}.$$

Now $W^{s,p}(U)$ is a Banach space. If $p = 2$, it is also a Hilbert space and it is usually denoted by $H^s(U)$.

2.4 The theory of ordinary differential equations

In section 2.1, the subject of study was the linear system $\dot{\mathbf{y}} = A\mathbf{y}$, where A was a matrix. More generally, consider the equation

$$\dot{\mathbf{y}} = F(\mathbf{y}) \tag{2.24}$$

where F could be non-linear and as usual $\dot{\mathbf{y}} = d\mathbf{y}/dt$. The properties of F will impact properties of the system, such as whether there is a unique solution or not. The system (2.24) is called autonomous, since F does not depend explicitly on t . A non-autonomous system is on the form $\dot{\mathbf{y}} = F(\mathbf{y}, t)$.

Example 2.1. Consider the 1-dimensional variable y and the mapping $F(y) = 3y^{2/3}$. Given the initial value $y(0) = 0$ and the ordinary differential equation $\dot{y} = 3y^{2/3}$, there is not a unique solution. Indeed, both $y = 0$ and $y(t) = t^3$ solve the equation and satisfy the initial condition.

The derivative $\dot{\mathbf{y}}$ is of first order, which might seem like a restriction, but higher order derivatives can be “removed” by the introduction of more variables. In section REF, the second order differential equation $y'' + by' + ay = 0$ that represents a damped oscillation on the position-variable y was reformulated as a system of first order equations:

$$\begin{aligned} \dot{y}_1 &= y_2 && \text{(velocity)} \\ \dot{y}_2 &= -by_2 - ay_1 && \text{(acceleration)} \end{aligned}$$

where a and b are constants. (The constants a and b are temporary in the sense that they will have a different meaning in possibly every paragraph.)

If there is a system of k equations of order ℓ , it is equivalent to a system of $k\ell$ first order equations.

The system (2.24) has a unique solution starting at $\mathbf{y}_0$ under certain conditions. A solution is a differentiable curve $\mathbf{y}(t)$, which maps t in some interval $a < t < b$ to a vector $\mathbf{y}(t)$ such that (2.24) is satisfied identically. Given a solution $\mathbf{y}$ of (2.24) defined on some open interval I_1 and another solution $\mathbf{x}$ defined on some open interval I_2 such that $I_1 \subsetneq I_2$, then $\mathbf{x}$ is called a proper extension of $\mathbf{y}$ if $\mathbf{x}(t) = \mathbf{y}(t)$ for all $t \in I_1$. If a solution curve has no proper extension, it is called a maximal solution.

Definition 2.1. If F maps from a normed linear space V_1 into another normed linear space V_2 then F is said to be continuous at $\mathbf{y} \in V_1$ if for all $\varepsilon > 0$ there exists a $\delta > 0$ such that $\mathbf{x} \in V_1$ and $\|\mathbf{x} - \mathbf{y}\| < \delta$ implies that

$$\|F(\mathbf{y}) - F(\mathbf{x})\| < \varepsilon.$$

Continuity of F is sufficient to ensure that (2.24) admits a solution, but it might not be unique. There is a stronger condition, which guarantees uniqueness:

Definition 2.2. Let U be an open subset of $\mathbb{R}^n$. A function $F : U \rightarrow \mathbb{R}^n$ is said to satisfy a Lipschitz condition on U if there is a constant $K > 0$ such that for all $\mathbf{y}, \mathbf{x} \in U$

$$\|F(\mathbf{y}) - F(\mathbf{x})\| \leq K\|\mathbf{y} - \mathbf{x}\|.$$

In particular the latter of the above definitions will help to solve the question about when there exists a solution to the initial value problem $\dot{\mathbf{y}} = F(\mathbf{y})$, $\mathbf{y}(0) = \mathbf{y}_0$. The following is the famous Picard-Lindelöf theorem, proving existence and uniqueness [8].

Theorem: If $F : E \rightarrow E$ satisfies a Lipschitz condition globally on E , $\|F(\mathbf{y}) - F(\mathbf{x})\| \leq K\|\mathbf{y} - \mathbf{x}\|$ for all $\mathbf{y}, \mathbf{x} \in E$, then given any $\mathbf{y}_0 \in E$, there exists a solution $\mathbf{y} : [0, \infty) \rightarrow E$ to the initial value problem $\dot{\mathbf{y}} = F(\mathbf{y})$, with initial data $\mathbf{y}(0) = \mathbf{y}_0$.

In the case of non-autonomous systems, $\dot{\mathbf{y}} = F(\mathbf{y}, t)$, the above theorem holds with a small modification. The Lipschitz condition is in that case usually not global. Local existence and uniqueness is however also interesting, and as the next theorem shows, a local solution continues to infinite time if there is no “blow up” scenario within finite time.

Theorem: If $F : U \times \mathbb{R} \rightarrow \mathbb{R}^n$ satisfies a Lipschitz condition on the first variable, there exists a maximal solution $\mathbf{y} : I \rightarrow E$ with $I = (a, b)$, and

- either $b = \infty$ or one has $\|\mathbf{y}(t)\| \rightarrow \infty$ as $t \rightarrow b_-$
- either $a = -\infty$ or one has $\|\mathbf{y}(t)\| \rightarrow \infty$ as $t \rightarrow a_+$.

Example 2.2. Consider $dy/dt = x^2$ with $y(0) = 1/b$, where $b > 0$ is a constant. Then

$$y(t) = \frac{1}{b - t}$$

and the maximal solution is defined on $t < b$, since $y(t) \rightarrow \infty$ as $t \rightarrow b$. Notice that $F(y) = y^2$ does not satisfy a Lipschitz condition globally on $\mathbb{R}$, but on bounded subsets of $\mathbb{R}$ it does.

A function $\phi : U \times I \rightarrow \mathbb{R}^n$ is called a flow if $\phi(x, 0) = x$ and $\phi(x, t + s) = \phi(\phi(x, s), t)$ whenever both sides of this equation are defined. In particular, if $t \mapsto \phi(x, t)$ is a family of solutions of the autonomous differential equation $\dot{x} = F(x)$ with $x(0) = x_0$ such that $\phi(\cdot, 0)$ is the identity mapping, then ϕ is a flow [13].

2.4.1 Linear stability analysis

A system of ODEs, $\dot{y} = w(y)$, where w is a function $\mathbb{R}^n \rightarrow \mathbb{R}^n$, with a stationary point y_0 may be analyzed close to the stationary point by Taylor expansion. Write $s = y - y_0$. Then $\dot{s} = \dot{y}$ and since y_0 is a stationary point $w(y_0) = 0$, so

$$\dot{s} \approx w(y_0) + Dw(y_0)(y - y_0) + \dots = Dw(y_0)s + \dots \quad (2.25)$$

Here, Dw is a square matrix. By the results in §2.1.2, the solution to the linear equation $\dot{s} = Dw s$ has components on the form

$$t^k e^{\lambda_j t}.$$

For such components, $|t^k e^{\lambda_j t}| \rightarrow 0$ when $t \rightarrow \infty$ if $\operatorname{Re}(\lambda_j) < 0$. Linear stability analysis of ODEs concludes that if the eigenvalues of Dw at y_0 has negative real parts then the perturbations s decay and the stationary point y_0 is stable.

2.4.2 ODEs on general Banach spaces

Much of the above theory applies to functions on Banach spaces in general. Consider a Banach space E and an open set U in E . A mapping $F : U \rightarrow E$ which is at least C^1 -smooth will be called a (time-independent) vector field on U . At each point on U , its value is interpreted as a vector. Let $u_0 \in U$. An integral curve for F with initial condition u_0 is a function $\alpha : I \rightarrow U$ which is at least C^1 -smooth and maps some open interval I onto a curve in U , solving

$$\alpha'(t) = F(\alpha(t)), \quad \text{with } \alpha(0) = u_0.$$

We state the Picard-Lindelöf theorem in the context of Banach spaces. The vector field F is said to satisfy a Lipschitz condition on U if there is a constant $L > 0$ such that

$$\|F(u) - F(v)\| \leq L\|u - v\| \quad \text{for all } u, v \in U.$$

Theorem: Let $F : U \rightarrow E$ satisfy a Lipschitz condition on U with constant $L > 0$. Let $u_0 \in U$, $0 < a < 1$ and assume that the closed ball of radius $2a$, $\bar{B}_{2a}(u_0)$ is contained in U , and that F is bounded by a constant $K > 0$ on this ball. If b is a positive number such that $b < a/K$ and $b < 1/L$, then there exists a unique local flow $\phi : B_a(u_0) \times (-b, b) \rightarrow U$ of F , that is, for each $u \in B_a(u_0)$ the map $\alpha : t \mapsto \phi(x, t)$ satisfies

$$\alpha'(t) = F(\alpha(t))$$

and $\alpha(0) = u$.

In order to prove this theorem, define the set of continuous maps from $[-b, b]$ into $\bar{B}_{2a}(u_0)$ starting at $u \in \bar{B}_a(u_0)$,

$$\alpha : [-b, b] \rightarrow \bar{B}_{2a}(u_0), \quad \alpha(0) = u.$$

This is a complete metric space when equipped with the supremum norm. Denote it by M and define the mapping T by

$$T\alpha(t) = u + \int_0^t F(\alpha(s)) ds.$$

Then $T\alpha$ is continuous and $T\alpha(0) = u$. Moreover,

$$\|T\alpha(t) - u\| \leq bK < a$$

so $T\alpha$ is bounded. Thus $T : M \rightarrow M$. It is also a contraction map, since for any two curves $\alpha, \beta \in M$,

$$\|T\alpha - T\beta\| \leq b \sup \|f(\alpha) - f(\beta)\| < bL\|\alpha - \beta\| < \|\alpha - \beta\|.$$

Therefore, there exists a fixed point $\alpha = T\alpha$, which proves the theorem.

Just like before, the “blow up” criterion holds for maximal solutions.

The flow of a vector field is as smooth as the vector field itself. That is, if the vector field F is of class C^p with $1 \leq p \leq \infty$, then the flow of F is also of class C^p on its domain of definition [47].

2.5 Differential geometry and Lie groups

A vector in $\mathbb{R}^n$ is typically represented by an n -tuple, where the i th coordinate in this tuple is the coefficient of the i th unit vector in $\mathbb{R}^n$. The i th unit vector is of course $e_i = (0, 0, \dots, 1, \dots, 0)$, that is, the vector with zeroes everywhere except at position i , where it is 1. The inner product in $\mathbb{R}^n$ is defined via $\langle e_i, e_j \rangle = \delta_{ij}$, where $\delta_{ij} = 0$ if $i \neq j$ and $\delta_{ii} = 1$. That is, for two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$,

$$\langle \mathbf{x}, \mathbf{y} \rangle = \sum_{i,j=1}^n x_i y_j \langle e_i, e_j \rangle = \sum_{i=1}^n x_i y_i. \quad (2.26)$$

The “length” of a vector $\mathbf{x}$ is defined as $\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$. In $\mathbb{R}^2$ there is an intuitive formula for the inner product of two vectors: Let θ be the angle between the vectors $\mathbf{x}$ and $\mathbf{y}$. Then $\langle \mathbf{x}, \mathbf{y} \rangle = \|\mathbf{x}\| \|\mathbf{y}\| \cos \theta$. In short, the

inner product gives the space the structure of geometry via distances and angles.

Euclidean geometry is based on the space $\mathbb{R}^n$ with the inner product (2.26). The idea in Riemannian geometry is to impose the Euclidean structure on sets locally (at every point). The circle, for example, can be equipped with coordinates and an inner product – but the coordinate expressions might change along the circle. Therefore, it is essential to differential geometry to define how coordinates transform over the sets. This is the motivation for the following definitions.

Given a set M , a chart on M is a subset U of M together with a bijective, continuous map $\phi : U \rightarrow \mathbb{R}^n$. Two overlapping charts (U, ϕ) and (V, ψ) are said to be compatible if $\phi(U \cap V)$ and $\psi(V \cap U)$ are open subsets of $\mathbb{R}^n$ and if the composite maps $\psi \circ \phi^{-1}$ and $\phi \circ \psi^{-1}$ are smooth. Charts provide $\mathbb{R}^n$ -coordinates on M and many properties are to be understood from their properties on $\mathbb{R}^n$. For instance, the smoothness of function f on M is defined via $f(\phi^{-1}(x))$ on a neighborhood of $x \in \mathbb{R}^n$. The composite maps $\psi \circ \phi^{-1}$ and $\phi \circ \psi^{-1}$ are change-of-coordinates mappings.

If the following two conditions are met, M is said to be a differentiable manifold: (a) The set M is covered by a set of charts. (b) M can be written as a union of compatible charts. Condition (b) defines what it means that there exists an *atlas* on M . If the charts map to $\mathbb{R}^n$ the manifold is called n -dimensional.

In the above construction, $\mathbb{R}^n$ is called the modeling space. To generalize the manifold concept to infinite dimensional modeling spaces, $\mathbb{R}^n$ is replaced by a topological vector space. Typical choices are Hilbert spaces, Banach spaces or Fréchet spaces. Further discussion about infinite-dimensional geometry will be postponed to the end of this chapter.

Let $\mathcal{F}_m$ be the set of smooth functions defined on a neighborhood of $m \in M$. If a linear map $v : \mathcal{F}_m \rightarrow \mathbb{R}$ satisfies the derivation property (Leibniz rule, or “the product rule”) at m ,

$$v(fg) = (vf)g(m) + f(m)(vg),$$

then v is called a tangent vector at $m \in M$. The tangent space of M at m is denoted by $T_m M$ and it is defined as the set of derivations of $\mathcal{F}_m$. In any chart (representing m) the coordinate expression for v is given by

$$vf = v^i \frac{\partial f}{\partial x^i}, \quad (2.27)$$

where $v^i = v(x^i)$ and x^i is the coordinate function that maps m to the i th coordinate of the chart. Given a differentiable curve $\gamma(t)$ on M such that $\gamma(0) = m \in M$, the curve defines a vector $v \in T_m M$ by $v = \dot{\gamma}(0)$, meaning that

$$vf = \left. \frac{d}{dt} f(\gamma(t)) \right|_{t=0}$$

and in components, $v^i = d\gamma^i/dt|_{t=0}$, where γ^i is the i th coordinate of γ . The tangent space $T_m M$ may therefore be defined as equivalence classes of curves sharing the same tangent vector at $m \in M$, and this agrees with the above definition of the tangent space.

Let φ be a C^1 -smooth map from a neighborhood U of $m \in M$ to a manifold N (which could be the same manifold M). The tangent map of φ at $m \in M$ is defined as the map [48]

$$\varphi_* : T_m M \rightarrow T_{\varphi(m)} N$$

given by relation $(\varphi_* v)(f) = v(f \circ \varphi)$ for any $f \in \mathcal{F}_{\varphi(m)}$. This map is sometimes called the push-forward of φ since it “pushes” the vector at $T_m M$ to a vector at $T_{\varphi(m)} M$. If φ is a bijective and invertible map such that also the inverse map φ^{-1} is differentiable, it is called a diffeomorphism.

The tangent bundle of M is the disjoint union

$$TM = \bigcup_{m \in M} \{m\} \times T_m M$$

together with a projection map $\pi : TM \rightarrow M$ onto the basepoint, that is, $\pi(v) = m$ for any $v \in T_m M$. The tangent bundle contains vector fields, which define vectors at each point $m \in M$. A vector field is a linear map from on the space of C^∞ -smooth functions on M such that this linear map satisfies the derivation property

$$v(fg) = gv(f) + fv(g).$$

A Riemannian metric on a differential manifold M is an inner product $g_m(,)$ on each tangent space $T_m M$ that may vary smoothly with the basepoint $m \in M$. That means that in a chart with coordinate $x^1, \dots, x^n$,

$$g_m \left(\frac{\partial}{\partial x^i}, \frac{\partial}{\partial x^j} \right) = g_{ij}(x^1, \dots, x^n)$$

is a smooth function. Equivalently, if u, v are vector fields on M , it is required that $m \mapsto g_m(u, v)$ is a smooth function on M .

Consider, for example, the product metric. Let M_1 and M_2 be two smooth manifolds with metrics g_1 and g_2 . The Cartesian product manifold, $M_1 \times M_2$, has a natural metric defined via the projections $\pi_1 : M_1 \times M_2 \rightarrow M_1$ and $\pi_2 : M_1 \times M_2 \rightarrow M_2$. Then

$$g_{(q,p)}(u, v) = g_q(d\pi_1 u, d\pi_1 v) + g_p(d\pi_2 u, d\pi_2 v)$$

for all $(q, p) \in M_1 \times M_2$ and $u, v \in T_{(q,p)}(M_1 \times M_2)$. Here, $d\pi_1$ and $d\pi_2$ are the tangent maps of π_1 and π_2 . The n -dimensional torus $\mathbb{T}^n$ with the metric here is called the *flat* torus.

A co-vector is a linear map $T_m M \rightarrow \mathbb{R}$. Co-vector fields are linear mappings of vector fields which are $\mathcal{F}$ -linear in the sense that a co-vector ω satisfies $\omega(fv) = f\omega(v)$ for $f \in \mathcal{F}(M)$ and a vector field v . It turns out that $\omega(v)(m)$ at a point $m \in M$ only depends on $v_m \in T_m M$. Rank 2 tensor fields of type $(0, 2)$ are bi-linear maps

$$TM \times TM \rightarrow \mathcal{F}(M),$$

which is $\mathcal{F}$ -linear in each variable. One important example on the Euclidean space $\mathbb{R}^n$ is the dot-product. Mixed tensor fields of type (r, s) are multilinear maps on r copies of the co-tangent bundle T^*M of co-vectors and s copies of the tangent bundle TM , see Ilisie [36] for details.

The differential of a function $f : M \rightarrow \mathbb{R}$ is a map df (the “differential of f ”) defined locally by $df_m(v) = vf$ for any vector $v \in T_m M$. The map df_m is linear on $T_m M$ and is called a co-vector or a 1-form. If f is smooth then df is a smooth co-vector field. The local coordinates of df are the partial derivatives (in a chart) of f . Define the map φ^* by $\varphi^*(df) = d(f \circ \varphi)$,

where φ is a diffeomorphism. This defines the so-called pullback map, which is the adjoint map of the push-forward map φ_* . The *Lie derivative* of a tensor field τ in direction of a vector field v is defined by

$$L_v \tau = \frac{d}{dt} \varphi_t^* \tau \Big|_{t=0}$$

where φ_t is the flow generated by v , that is, the solution to $\dot{\varphi} = v \circ \varphi$.

Given a Riemannian metric g and a vector field v , a corresponding 1-form $g(v, \cdot)$ is defined by the mapping $u \mapsto g(v, u)$. The components of the 1-form of v are usually written as v_i . Consequently, the inner product of two vector fields u and v , via the metric g can be written as $u^i v_i$, where the summation over i is understood. This is the so-called Einstein notation. For a 1-forms ω with components ω_i , the corresponding vector field has the components $\omega^i = g^{ij} \omega_j$, where (g^{ij}) is the inverse matrix of (g_{ij}) . The metric extends to tensors of type (r, s) by

$$g(Q, P) = g_{i_1, j_1} \dots g_{i_r, j_r} g^{k_1, l_1} \dots g^{k_s, l_s} Q_{k_1, \dots, k_s}^{i_1, \dots, i_r} P_{l_1, \dots, l_s}^{j_1, \dots, j_r}$$

The tangent map φ_* defines a transport of the metric called the pushforward metric. It is given by

$$(\varphi_* g)_p(u, v) = g_{\varphi^{-1}(p)}(d\varphi^{-1}u, d\varphi^{-1}v)$$

for any $u, v \in T_p M$.

The *gradient* of a function f on M is the unique vector field ∇f that satisfies

$$df(v) = g(\nabla f, v) \quad \text{for all vector fields } v \in TM.$$

The gradient in Euclidean coordinates coincides with the gradient from elementary calculus.

A k -form on a manifold M is a $(0, k)$ -tensor which is antisymmetric under the exchange of any pair of indices. The space of k -forms on M is denoted by $\Omega^k(M)$. The so-called wedge product of a k -form ω and an l -form η is denoted by $\omega \wedge \eta$. As a product, it is associative and bilinear, and it satisfies the commutation relation $\omega \wedge \eta = (-1)^{kl} \eta \wedge \omega$. If ω is defined on

an open subset U of $\mathbb{R}^n$ then it can be written using the wedge product of the differentials dx^i ,

$$\omega_x = \phi(x) dx^1 \wedge dx^2 \wedge \dots \wedge dx^n,$$

where $\phi : U \rightarrow \mathbb{R}$ is a function. The integral of ω is then defined as

$$\int_U \omega = \int_U \phi(x) dx^1 dx^2 \dots dx^n.$$

One proceeds to defined the integral over M by means of an atlas on M and partition on unity [48]. The Riemannian metric induces an n -form, which in local coordinates is

$$\mu_g = \sqrt{\det(g_{ij})} dx^1 \wedge \dots \wedge dx^n.$$

Here, $\det(g_{ij})$ is the determinant of the metric in coordinates.

2.5.1 Affine connection, tensors

A *vector bundle* over a topological space M is a topological space E with a surjective, continuous map $\pi : E \rightarrow M$ that satisfies (a) the fiber $E_m = \pi^{-1}(m)$ has the structure of a vector space, and (b) there exists a local trivialization of E over any neighborhood U around $m \in M$. One special vector bundle is the tangent bundle TM over a smooth manifold M . A *section* of a vector bundle $\pi : E \rightarrow M$ is a continuous map $f : M \rightarrow E$ such that $\pi(f(m)) = m$ for all $m \in M$. Then, a vector field on M is a section of the tangent bundle of M . The set of all smooth (global) sections of a vector bundle is a vector space under pointwise addition and scalar multiplication [48]. The set of smooth sections of a vector bundle $\pi : E \rightarrow M$ is usually denoted by $\Gamma(E)$, except for some sections of special importance, like the vector fields.

Let $\mathfrak{X}(M)$ be the set of C^∞ -smooth vector fields on M . An affine connection is a mapping

$$\nabla : \mathfrak{X}(M) \times \mathfrak{X}(M) \rightarrow \mathfrak{X}(M)$$

which is denoted $(u, v) \mapsto \nabla_u v$ and satisfies the following properties: For any smooth functions $f, g \in \mathcal{F}(M)$ and any vector fields $u, v, w \in \mathfrak{X}(M)$,

- (i) $\nabla_{f u + g v} w = f \nabla_u w + g \nabla_v w$
- (ii) $\nabla_u(v + w) = \nabla_u v + \nabla_u w$
- (iii) $\nabla_u(f v) = f \nabla_u v + u(f) v$

In other words, $\nabla_u v$ is a vector fields depending linearly on u and v . The affine connection is $\mathcal{F}$ -linear in the first variable. It can be extended to tensor fields, which leads to the notion of curvature and torsion (see Straumann [74]).

Let γ be a differentiable curve on M . There exists a correspondence between a vector field v along γ and another vector field, Dv/dt , along the same curve such that

- (i) $\frac{D}{dt}(u + v) = \frac{Du}{dt} + \frac{Dv}{dt}$
- (ii) $\frac{D}{dt}(f v) = f \frac{Dv}{dt} + \frac{df}{dt} v$
- (iii) If v is induced by a vector field w , that is $v(t) = w(\gamma(t))$, then $\frac{Dv}{dt} = \nabla_{d\gamma/dt} w$.

The vector field $\frac{Du}{dt}$ is called the covariant derivative [16] of u along γ . The curve γ is called a geodesic of the connection ∇ if $\dot{\gamma}$ is parallel along γ , that is $D\dot{\gamma}/dt = 0$. Geodesics are optimal paths in the sense that they minimize *arc length*. The arc length of a curve γ that joins the points $\gamma(a)$ and $\gamma(b)$ is given by $\int_a^b \sqrt{g(\dot{\gamma}, \dot{\gamma})} dt$. Conversely, if a piecewise differentiable curve minimizes arc length, then it is a geodesic.

Let g be a metric on M . A connection on M is said to be compatible with the metric if for any smooth curve γ the following holds: given any two vectors u, v along γ , the inner product $g(u, v)$ is constant along γ . The motivation for this definition is that there follows a “product rule”

$$\frac{d}{dt} g(u, v) = g\left(\frac{Du}{dt}, v\right) + g\left(u, \frac{Dv}{dt}\right)$$

if and only if the connection is compatible with the metric.

A connection ∇ on M is said to be symmetric if it satisfies $\nabla_u v - \nabla_v u = [u, v]$ for any two vector fields u, v . If a Riemannian metric is given, there exists a

unique connection that is both symmetric and compatible with the metric. Such a connection is called a Levi-Civita connection.

The space of smooth vector fields, $\mathfrak{X}(M)$, can be equipped with the inner product

$$\langle u, v \rangle = \int_M g(u, v) \mu_g.$$

Similarly, for (r, s) -tensor fields the inner product is $\int_M g(Q, P) \mu_g$ and in even more generality, if $(\cdot, \cdot)$ is an inner product on fibers of a vector bundle, $\int_M (u, v) \mu$ for some volume form μ is an inner product on (global) sections on the vector bundle. Let T be a differential operator $T : \Gamma(E) \rightarrow \Gamma(F)$ between sections of vector bundles E and F . A pair of differential operators T and T^* are called formally conjugate if

$$\int_M (Tu, v) \mu = \int_M (u, T^*v) \mu.$$

For example, define the covariant divergence δ_g on the space of symmetric $(0, 2)$ -tensors by the local coordinate expression $\delta_g(h)^i = \nabla_j h^{ij}$. Here, ∇_j is the coordinate expression of the covariant derivative in the direction of the vector $\partial/\partial x^j$. Then consider the *Lie derivative* L_v in the direction of the vector field v applied to the space of $(0, 2)$ -tensor fields. If ∇ is the Levi-Civita connection associated with g , then $L_v g = \nabla_i v_j + \nabla_j v_i$. Define $\ell_g : v \mapsto -\frac{1}{2} L_v g$. In this case, by Stokes' theorem [48],

$$\int_M g(\delta_g h, v) \mu_g = \int_M g(h, -\frac{1}{2} L_v g) \mu_g$$

that is $\langle \delta_g h, v \rangle = \langle h, \ell_g v \rangle$, so δ_g is formally conjugate to ℓ_g .

2.5.2 Lie groups

A set of smooth transformations of a manifold M into M itself is called a group, usually denoted by G , if the following conditions are met:

1. For all $g, h \in G$, the composition $g \circ h$ belongs to G .
2. There exists an inverse map, g^{-1} , to every $g \in G$ which also belongs to G .

It follows that every group contains the identity transformation (the unit), usually denoted by e . A Lie group is a group such that the above operations are smooth.

Example 2.3. Consider $n \times n$ real matrices that are invertible, with the regular multiplication of matrices and the identity matrix as given in section 2.1. This set of matrices and their multiplication is called the general linear group $GL(n, \mathbb{R})$.

A (real) Lie algebra, X , is a real vector space together with a bi-linear map called the Lie bracket on X , denoted by $[\cdot, \cdot]$, such that the following identities hold:

- $[\xi, \xi] = 0$ for any $\xi \in X$
- (Jacobi identity) For all $\xi, \eta, \zeta \in X$,

$$[\xi, [\eta, \zeta]] + [\zeta, [\xi, \eta]] + [\eta, [\zeta, \xi]] = 0.$$

The tangent space to the Lie group at $e \in G$ is called the vector space of the Lie algebra and it is usually denoted by $\mathfrak{g}$. It receives its algebraic structure from the vector commutator $[\xi, \eta] = \xi\eta - \eta\xi$.

A Lie group G can act on a manifold Q . That is, elements of G can transform points on Q . Denote by $g \cdot q$ the action of $g \in G$ on $q \in Q$. By definition, a *left action* of a Lie group is a smooth map of a pair $(g, q) \in G \times Q$ to an element $g \cdot q \in Q$ such that (i) the identity transformation $e \in G$ leaves q unchanged and (ii) if $g, h \in G$ are two transformations then $gh \cdot q = g \cdot (h \cdot q)$, where gh is the composition $g \circ h$. A *right action* of a Lie group G on Q is denoted by $q \cdot g$ and instead of the second condition, the composition gh acts on Q following the opposite order: gh applied to q equals first acting on q with g and then with h .

For example, a Lie group acts on itself by composition from the left or right. Denote by L_g the map $L_g h = gh$ and let R_g be the map $R_g h = hg$. These maps are, respectively, left and right actions. Another example of an action is the action of $GL(n, \mathbb{R})$ on $\mathbb{R}^n$ from the left by the regular matrix multiplication, that is $(A, v) \mapsto Av$.

The mapping $R_{g^{-1}}L_g$ on G defined by $h \mapsto ghg^{-1}$ is a diffeomorphism on G . Its derivative at the identity is a linear map from the vector space of the Lie algebra to itself. It is usually denoted by $\text{Ad}_g : \mathfrak{g} \rightarrow \mathfrak{g}$. This map induces a map $\text{Ad} : g \mapsto \text{Ad}_g$ called the adjoint representation of the group. It maps group elements of G into $GL(\mathfrak{g})$, the Lie group of all bijective linear maps on $\mathfrak{g}$. The derivative of Ad at the identity is a mapping of vectors, $\text{ad} : \mathfrak{g} \rightarrow \mathfrak{gl}(\mathfrak{g})$, where $\mathfrak{gl}(\mathfrak{g})$ is the Lie algebra of linear maps from $\mathfrak{g}$ to itself. For a linear group, it can be verified that

$$\text{ad}_\xi(\eta) = [\xi, \eta].$$

An action is said to be

- transitive if for every two points on Q , say q and q' , there is a transformation $g \in G$ such that $g \cdot q = q'$,
- effective (or faithful) if only the identity transformation $e \in G$ defines the identity action, and
- free if for every $q \in Q$, if $g \cdot q = q$ then $g = e$.

The *orbit* of a group action starting at q is the set $G \cdot q = \{g \cdot q : g \in G\} \subset Q$. The so-called group adjoint orbits of the group G are the orbits of the Ad -action in the Lie algebra.

The mapping ad has a corresponding dual map defined on the dual of the Lie algebra, $\mathfrak{g}^*$. The dual $\mathfrak{g}^*$ is the space of linear, real functionals on the Lie algebra. One defines left and right translation maps, L_g^* and R_g^* , via their actions on the primal space $\mathfrak{g}$:

$$L_g^* \tau(\xi) = \tau(g \cdot \xi), \quad R_g^* \tau(\xi) = \tau(\xi \cdot g),$$

where $g \cdot \xi$ is the tangent map of the left multiplication applied to ξ and $\xi \cdot g$ is the tangent map of the right translation. Similarly, Ad^* is defined¹ via $\text{Ad}_g^* \tau(\xi) = \tau(\text{Ad}_g \xi)$, and the Ad^* operator satisfies $\text{Ad}_{gh}^* = \text{Ad}_h^* \text{Ad}_g^*$ for all $g, h \in G$. Thus it forms a representation, which is called the co-adjoint representation. The Ad^* action on $\mathfrak{g}^*$ produces the co-adjoint orbits of

¹These definitions might be subject to sign conventions [44].

G . Moreover, $\text{ad}_\eta^* \tau(\xi) = \tau(\text{ad}_\eta \xi)$. The mapping $\text{ad}_\xi^* : \mathfrak{g}^* \rightarrow \mathfrak{g}^*$ is a linear operator on the dual space to the algebra [2].

Unfortunately, the dual space of a Fréchet space is not necessarily a Fréchet space and the co-adjoint actions could be degenerate. The analysis in this case can be conditioned on the dual space to ensure the appropriate properties of the dual space (for instance, that the co-adjoint action is uniquely determined by $\text{Ad}_g^* \tau(\xi) = \tau(\text{Ad}_g \xi)$). The resulting subspace is usually called the “smooth duals” [44].

Left translation on a Lie group defines a left-invariant metric via the inner product on the Lie algebra. The metric at any $g \in G$, denoted by $\langle\langle u, v \rangle\rangle_g$ is determined by translation of the vectors $u, v \in T_g G$ to the tangent space at the identity element $e \in G$,

$$\langle\langle u, v \rangle\rangle_g = \langle\langle \xi, \eta \rangle\rangle_e, \quad u = g \cdot \xi, \quad v = g \cdot \eta.$$

Here, $g \cdot \xi$ is the tangent map of the left translation map L_g . Completely analogous is the construction of a *right*-invariant metric on G . In general, a Riemannian metric $\langle\langle \cdot, \cdot \rangle\rangle : TG \times TG \rightarrow \mathbb{R}$ on G is called *right-invariant* if

$$\langle\langle \xi, \eta \rangle\rangle_e = \langle\langle \xi \cdot g, \eta \cdot g \rangle\rangle_g, \quad \forall g \in G, \quad \forall \xi, \eta \in \mathfrak{g},$$

where $\xi \cdot g$ denotes the tangent lifted right action of g on ξ . Next, let $\langle, \rangle$ be the inner product on $\mathfrak{g} = T_e G$ and let A be a differential operator such that it is symmetric in the inner product on $\mathfrak{g}$, that is $\langle A\xi, \eta \rangle = \langle A\eta, \xi \rangle$ for all $\xi, \eta \in \mathfrak{g}$. If A is a positive, symmetric, bijective pseudo-differential operator, the above inner product can be defined by $\langle\langle \xi, \eta \rangle\rangle_e = \langle A\xi, \eta \rangle$. With A , one associates a linear mapping of vectors in $\mathfrak{g}$ defined via $\xi \mapsto \langle A\eta, \xi \rangle$. This provides an identification of $A\eta$ with an element of $\mathfrak{g}^*$ and we write $A : \mathfrak{g} \rightarrow \mathfrak{g}^*$.

For example, consider the motion of a rigid body that is rotating around some fixed point. Then the configuration of the body is determined by the angles of rotation. Euler rightly figured out that the rotations of a rigid body have a group structure. The group is $\text{SO}(3)$, as any rotation in $\mathbb{R}^3$ can be represented by an orthogonal matrix with determinant +1. Let ω be the angular velocity of the body and $\mathbf{m}$ its angular momentum. If ω and

$\mathbf{m}$ are expressed in components with respect to the principal axes of the rotating body, they are related via the moment of inertia matrix

$$A = \begin{bmatrix} I_1 & 0 & 0 \\ 0 & I_2 & 0 \\ 0 & 0 & I_3 \end{bmatrix}$$

and $\mathbf{m} = A\boldsymbol{\omega}$. The constants I_1, I_2 and I_3 depend only on the shape and mass distribution of the rigid body and they represent the inertia of rotation. The rotational energy is $E(\boldsymbol{\omega}) = \langle \boldsymbol{\omega}, A\boldsymbol{\omega} \rangle$, where the inner product is the usual dot product. The Lie algebra of $\text{SO}(3)$ is denoted by $\mathfrak{so}(3)$ and consists of all skew-symmetric 3×3 matrices, which are “infinitesimal generators of rotation”. If a small rotation by an angle θ occurs about the axis (x, y, z) , then the rotation matrix can be represented as

$$R_\theta = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \theta \begin{bmatrix} 0 & -z & y \\ z & 0 & -x \\ -y & x & 0 \end{bmatrix}.$$

The Lie algebra is therefore identified with $\mathbb{R}^3$ via the “hat isomorphism”

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \boldsymbol{\omega} \mapsto \hat{\boldsymbol{\omega}} = \begin{bmatrix} 0 & -z & y \\ z & 0 & -x \\ -y & x & 0 \end{bmatrix}.$$

Via this identification of $\mathfrak{so}(3)$ with $\mathbb{R}^3$, the Lie bracket on $\mathfrak{g}$ is the vector cross product $[\mathbf{u}, \mathbf{v}] = \mathbf{v} \times \mathbf{u}$. The *Euler-Arnold* equation [44] gives the equations of motion in terms of $\mathbf{m} = A\boldsymbol{\omega}$:

$$\dot{\mathbf{m}} = \mathbf{m} \times A^{-1}\mathbf{m}.$$

The generalization of momenta to an abstract group setting is provided by the so-called *momentum mapping*. Given a left action $g \cdot q$ on a configuration $q \in Q$, the infinitesimal action is the tangent map of the action map at the identity $e \in G$. It is denoted $v \cdot q$, where $v \in \mathfrak{g}$. Lifting this to the dual gives the cotangent lifted momentum map of the left action:

$$J : T^*Q \rightarrow \mathfrak{g}^*, \quad \langle J(q, p), v \rangle = \langle p, v \cdot q \rangle.$$

Here, the pairings and the group actions define the momentum mapping J . The infinitesimal generator of the $\text{SO}(3)$ action on $\mathbb{R}^3$ is given by $\hat{\omega}q = \omega \times q$, and with the dot product pairing, $\langle J(q, p), \omega \rangle = \langle p, \hat{\omega}q \rangle = \langle \omega, q \times p \rangle$, that is,

$$J(q, p) = q \times p.$$

Thus, in classical mechanics description of a rigid body, the momentum map of the rotation group action is the angular momentum vector [49, 35].

One group of particular importance to Paper III is the group of diffeomorphisms on a compact² n -dimensional manifold M . Denote by $\mathcal{D}(M)$ the smooth diffeomorphisms on M . It is an open subspace of all smooth maps from M to M , which is a Fréchet manifold. It is a Lie-Fréchet group [31] under the composition map (both the composition map and the inversion map are smooth). The Lie algebra of $\mathcal{D}(M)$ is the set of smooth vector fields on M with the usual vector field commutator. On (infinite-dimensional) Fréchet manifolds, tangent spaces and vector fields are defined as in the usual finite-dimensional case, see Khesin and Wendt [44], with some notable exceptions [9]. Therefore, the group of smooth diffeomorphisms on M is suitable for a geometric treatment. However, several analytical tools are lost on Fréchet manifolds, such as the inverse function theorem and the fixed point theorem. Some of the implications cause deep problems for existence of solutions to certain differential equations. The exponential map, for instance, is the time-one solution to the following ordinary differential equation: Let $\tilde{v}$ be the left-invariant vector field $\tilde{v} = g \cdot v$ for some $v \in \mathfrak{g}$. If it exists, the flow ϕ_v is a map $G \times \mathbb{R} \rightarrow G$ that satisfies

$$\frac{\partial}{\partial t} \phi_v(g, t) = \tilde{v}(\phi_v(g, t))$$

with $\phi_v(g, 0) = g$. Then, the exponential map $\exp : \mathfrak{g} \rightarrow G$ is defined as $v \mapsto \phi_v(e, 1)$. In order to re-gain control of such analytical tools, it is convenient to set up a larger group of diffeomorphisms: the Sobolev class diffeomorphisms.

²The group of diffeomorphisms on a non-compact manifold is not complete [44].

2.5.3 Sobolev class diffeomorphisms

Here, we follow the presentation by Ebin and Marsden [21]. Based on Arnold's [1] geometric description of hydrodynamics, Ebin and Marsden developed analysis tools that enabled a set of existence and uniqueness results (see [41, 4, 42] for modernized developments).

Let M be a compact, smooth, oriented manifold possibly with smooth boundary, and let $\pi : E \rightarrow M$ be a vector bundle over M . Define the Hilbert space $H^s(E)$ of sections of E whose distributional derivatives up to order s are square integrable (in charts). Let $C^k(E)$ be the space of sections of E of class C^k . This is a Banach space under a norm which induces the topology of uniform convergence of all derivatives of order less than k . Also, $C^k(E)$ is the completion of $C^\infty(E)$ under this norm. By the Sobolev embedding theorem, for $s > \frac{1}{2} \dim M + k$, where k is non-negative, the space $H^s(M)$ is continuously included in $C^k(M)$.

If M and N are compact manifolds and $s > \frac{1}{2} \dim M$ then consider the space $H^s(M, N)$ of H^s maps from M to N . Similarly, the Banach manifold $C^k(M, N)$ is defined. The set $C^1\mathcal{D}(M)$ of C^1 -diffeomorphisms on M is open in $C^1(M, M)$ and is a topological group under the composition map. Define the group of H^s -diffeomorphisms as $\mathcal{D}^s(M) = H^s(M, M) \cap C^1\mathcal{D}(M)$. It is an open set, a topological group and

$$\mathcal{D}^s(M) = \{\varphi \in H^s(M, M) : \varphi \text{ is bijective and } \varphi^{-1} \in H^s(M, M)\}.$$

Since $\mathcal{D}^s(M) \subset H^s(M, M)$ is open, $T_e\mathcal{D}^s(M)$ is the space of all H^s vector fields on M . Here, $e \in \mathcal{D}^s(M)$ is the identity mapping on M .

The group of H^s -diffeomorphisms is a topological group because not all group actions are smooth. The inversion map $\varphi \mapsto \varphi^{-1}$ is continuous, but not smooth. The right composition map $R_\psi : \varphi \mapsto \varphi \circ \psi$ is smooth. However, the left composition map $L_\psi : \varphi \mapsto \psi \circ \varphi$ is continuous, but not even Lipschitz continuous [20]. In general, if $\psi \in H^{s+l}(M, N)$ defines a map $\omega_\psi : \varphi \mapsto \psi \circ \varphi$ then ω_ψ is a C^l -map. This is known as the “omega lemma.”

Theorem: (*Theorem 3.1 of Ebin and Marsden [21].*) Let M be a compact

n -dimensional manifold without boundary and $s > (n/2) + 2$. Then, if v is an H^s vector field on M , its integral curve α is a C^1 curve on $\mathcal{D}^s(M)$ and a one-parameter subgroup of $\mathcal{D}^s(M)$. Moreover, the exponential map $v \mapsto \alpha(1)$ is continuous, but not C^1 .

From the omega lemma we get that if v is H^{s+l} , the integral curve is C^{l+1} -smooth.

In order to retrieve the smooth C^∞ topology of the diffeomorphism group, define the smooth diffeomorphisms by

$$\mathcal{D}(M) = \bigcap_{s > n/2} \mathcal{D}^s(M).$$

This groups is an inverse limit Hilbert group [63]. Both composition and inversion are smooth mappings on $\mathcal{D}(M)$, which recovers the group of diffeomorphisms as a Lie group. Its Lie algebra is the space of smooth vector fields, $\mathfrak{X}(M)$ with the usual bracket [21].

3

Decision-making and disease outbreaks

We have it under control. It's going to be just fine.

—Donald Trump (in a CNBC interview Jan 22, 2020)

How many people will be infected during a disease outbreak within, say, a week, given the current conditions such as the number of infected individuals and transmission rates? These types of questions are effectively answered by dividing the population into *compartments* (or categories) such as “susceptible” and “recovered”. The flow of people between compartments model the process of catching a disease and recovery, and in more advanced models, it can describe vaccinations, incubation times, etc. [17] Mathematically, we solve a non-linear initial value problem. Theoretically, we contribute to the understanding of what drives the spreading of diseases. This chapter introduces some of the standard models and presents our contribution to the field.

The COVID-19 pandemic outbreak in the beginning of 2020 issued many questions about people's behavior during disease outbreaks, such as “What difference does it make if *this large* a portion of the population complies with recommendations while the rest do not?” My supervisor and I incorporated ideas from game theory with the disease spreading models SIR and SIS in order to provide some insights to these questions. We realized that the individual decisions during a pandemic resemble the prisoner's

dilemma (PD) game and we investigated what happens when the population is under the influence of the PD game while also being aware of the risk of catching the disease. It was discovered how cooperation emerges when the game's payoff is a trade-off between the PD and the effect on disease spreading through changes to the infection transmission rate.

3.1 Modeling disease outbreaks

Some diseases confer immunity after an infection, while some do not. Immunity can last very long, sometimes as long as a lifetime, and sometimes much shorter. Examples of the former is the measles [78]. Common colds and many STIs are examples of diseases that do not confer immunity; it is probable that one can catch the disease again almost immediately after recovery [59, 81].

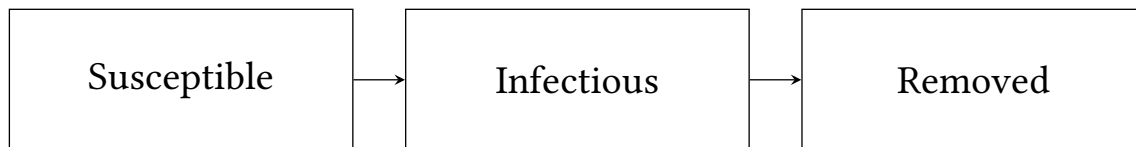
3.1.1 The SIR model

The following model was an early attempt at describing the dynamics among the population during an outbreak of a disease that confers lifetime immunity or immediate death. Assume that the population is divided into three categories, each consisting of individuals that are in one of the following states:

- Susceptible
- Infectious
- Removed (dead or immune)

Denote by S , I and R the number of susceptible, infectious and removed individuals, respectively. The model cannot differentiate between dead and immune because both types mean that the individual – dead or immune – does not participate in the disease spreading. Let N denote the size of the population, so that $S + I + R = N$. Dynamics in this model are captured by the change of state within the population, that is if, say, a susceptible individual gets sick then it moves to compartment I and correspondingly there would be an increase by 1 of I while S decreases by 1.

The classic SIR model assumes that all individuals in the population has equal probability to get in contact with any of the other individuals. It further introduces the probability of disease transfer from an infectious individual to a susceptible individual as a positive parameter β . This parameter can vary with time. The number of susceptible individuals can only decrease since the infected individuals eventually become removed (by death or – hopefully – by becoming immune). At each time, the expected decrease is proportional to the risk of a susceptible individual meeting with an infectious individual, that is, S would decrease by βSI . Let $S(t_k)$ be the number of susceptible individuals at time t_k . Then $S(t_{k+1}) - S(t_k) = \beta S(t_k)I(t_k)$ would describe this situation.¹



In large populations, it is usually feasible to approximate the integer numbers S , I and R with continuous real values. Therefore we describe the dynamics of S by means of the ordinary differential equation $\dot{S} = -\beta SI$, where the dot over S means differentiation with respect to the time variable. Then the flow scheme above says the the amount subtracted from S should be added to the compartment I . The rate at which individuals transfer to the removed state is such that $\dot{R} = \gamma I$ for a constant $\gamma > 0$. We obtain

$$\dot{S} = -\beta SI \quad (3.1)$$

$$\dot{I} = \beta SI - \gamma I \quad (3.2)$$

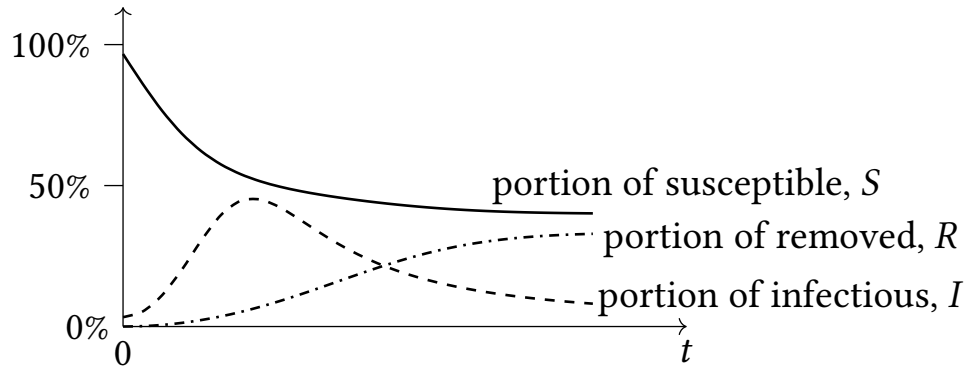
$$\dot{R} = \gamma I \quad (3.3)$$

Notice that $\dot{S} + \dot{I} + \dot{R} = 0$ meaning that the size of the population is constant. This assumption is realistic for many common diseases as the number of deaths are not usually changing the population size very much. The birth rate is assumed to be negligible or effectively the same as the death rate.

A sketch of typical time dynamics in the SIR model is pictured below. The

¹Notice that β is dimensionless, although, since each timestep is indexed, we may argue that it has dimensions 1/(time).

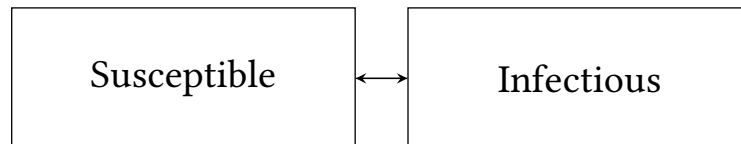
portion of susceptible individuals (full line) decreases as the portion of infectious (dashed line) increases during the outbreak of the disease. After some time, there is a portion of removed individuals (dashed dotted line). The dynamics stabilize after long time to a *steady state* with no infectious individuals. Notice that there might be susceptible individuals at steady state, because with $I = 0$ there is no flow between the compartments.



If we rewrite (3.2) as $\dot{I} = (R_0 S - 1)\gamma I$ with $R_0 = \beta/\gamma$ we see that the ratio R_0 determines whether there is a disease outbreak at small times. Above it is assumed that $R_0 S(0) > 1$ because otherwise there would be no increase of I at small times.

3.1.2 The SIS model

Instead of being “removed” as in the SIR model we may assume that recovery from the disease is immediately followed by the risk of catching the same disease again. In other words, recovery from the disease does not infer immunity for the individual. This situation is correctly modeled if the recovered individuals flow back to the susceptible compartment.



That is, the portion γI is added at each time to the change of S , giving $\dot{S} = -\beta SI + \gamma I$. In total,

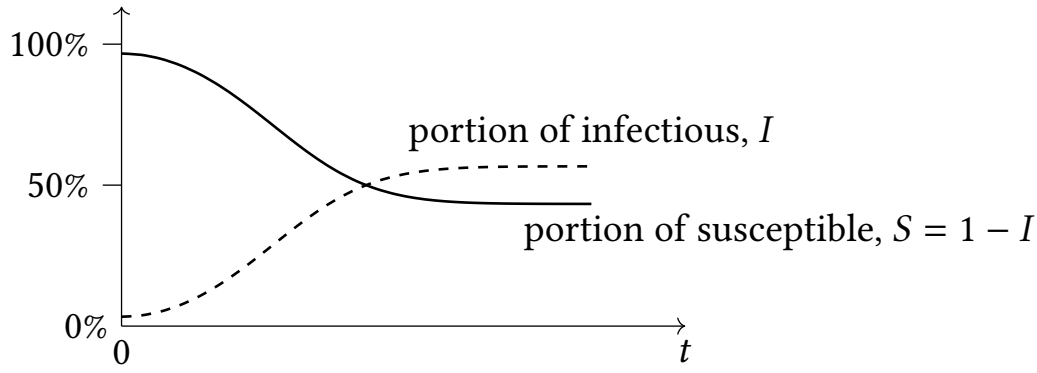
$$\dot{S} = -\beta SI + \gamma I$$

$$\dot{I} = \beta SI - \gamma I$$

Since $S + I = 1$ in this situation, we can eliminate S from the equations. The full dynamics is described by

$$\dot{I} = \beta(1 - I)I - \gamma I \quad (3.4)$$

A sketch of typical time dynamics in the SIS model is pictured below. The portion of susceptible (full line) decreases as the number of infectious (dashed line) increases during the outbreak of the disease. After some time, the dynamics stabilize to a *steady state* which is characterized by a balance between recovery and infection, that is, $\beta SI = \gamma I$.



Using (3.4) we compute

$$\frac{d}{dt} \frac{1}{I} = -\frac{\dot{I}}{I^2} \implies \frac{d}{dt} \frac{1}{I} + (\beta - \gamma) \frac{1}{I} = \beta. \quad (3.5)$$

If $\beta \neq \gamma$ then

$$I(t) = \frac{\beta - \gamma}{v_0 e^{-(\beta - \gamma)t} + \beta} \quad (3.6)$$

for some $v_0 \in \mathbb{R}$ (see Hethcote [33] for the same result with different notations). If $\beta = \gamma$ then $I(t) = 1/(\beta t + w_0)$ for some $w_0 \in \mathbb{R}$. If $\beta > \gamma$ then $I(t) \rightarrow 1 - \gamma/\beta$ as $t \rightarrow \infty$ and if $\beta \leq \gamma$ then $I(t) \rightarrow 0$ as $t \rightarrow \infty$. The ratio between β and γ plays an important role in the dynamics, similar to the case of the SIR model.

3.1.3 More complex models

There is vast literature on more advanced models than the ones outlined above. For instance, one may assume that there is an incubation period

for the disease. Then the susceptible individuals will not contribute to the disease spreading immediately after becoming infected, so there is a time delay between catching the disease and moving to the compartment I . Further examples of models are found in, e.g., Vynnycky and White [77].

3.2 The game theoretical beta-parameter

In the previous section we encountered the equations of the SIR model and the SIS model, which both assume that there is a infection rate β such that βSI is the portion of susceptible individuals that catch the disease at each timestep. The parameter β need not be constant. In our work, we have assumed that some individuals in the population are more effective at disease spreading, meaning that we associate a larger infection rate to them. We denote those individuals by D and the rest get the label C , so that β_D is the infection rate of individuals of class D and β_C is the infection rate of individuals of class C . By assumption $\beta_C < \beta_D$. Let β be the average over the population, that is if x is the portion of C -individuals then

$$\beta = x\beta_C + (1 - x)\beta_D. \quad (3.7)$$

Assuming that the infection rate is determined by individual *choice*, we may interpret D as the game theoretic strategy “defection”. Similarly, C stands for “cooperation”.

In order to model trends in the choice between cooperation and defection within the population, we assumed that the portion x is governed by a replicator’s equation. The payoffs that each individual perceive is assumed to be a balance between contributing to the common good (by cooperating) or gaining personal benefits (by defecting). In this situation x depends on time and we write $x = x(t)$.

By interpreting x as the portion of cooperators there is a flow of the defectors becoming cooperators given by

$$\dot{x} = \alpha x(1 - x)(\beta_D - \beta_C)I, \quad (3.8)$$

where $\alpha \geq 0$ is a parameter. The factor $x(1 - x)$ ensures that x remains in the range $0 \leq x \leq 1$. We may interpret (3.8) as a risk assessment managed by each individual: If there are many more infectious individuals that do not cooperate, then there is more risk of catching the disease and more individuals will decide to cooperate, that is, x will increase.

3.2.1 The combined SIR-PD and SIS-PD models

We would like to consider the total contribution of (3.8) and (2.20). Notice that both equations are on the same form as (2.17). Individuals are assumed to consider the total cost as the sum of $-\alpha(\beta_D - \beta_C)I$ and $C - N(k)$. The portion x is thus determined by the choices of individuals making conscious decisions based on the risk of catching the disease on the one hand, and on the other hand the benefits of the PD-game. These decisions determine the total transmission rate of the disease, which the entire population experiences. In the SIR-PD model,

$$\dot{S} = -((1 - x)\beta_D + x\beta_C)SI \quad (3.9)$$

$$\dot{I} = ((1 - x)\beta_D + x\beta_C)SI - \gamma I \quad (3.10)$$

$$\dot{R} = \gamma I \quad (3.11)$$

$$\dot{x} = x(1 - x)(\alpha(\beta_D - \beta_C)I - (C - N(k))) \quad (3.12)$$

whereas in the SIS-PD model,

$$\dot{I} = ((1 - x)\beta_D + x\beta_C)(1 - I)I - \gamma I \quad (3.13)$$

$$\dot{x} = x(1 - x)(\alpha(\beta_D - \beta_C)I - (C - N(k))) \quad (3.14)$$

Notice that the portion of cooperators is influenced by I which is itself dynamic. This results in a feedback mechanism. If a member of the population decides to change strategy from defect to cooperate, then the effective disease transmission rate (3.7) is decreased which causes I to shrink which in turn causes x to increase. Nevertheless, there are steady state solutions to the SIR-PD model and the SIS-PD model as we will see in the next section.

The parameter α balances the contribution from the term $(\beta_D - \beta_C)I$ with that of the term $C - N(k)$. We interpret this as a timescale difference. If

an individual gets updates on the portion of infectious, I , on the timescale “days” whereas the PD game payoff can be received on the timescale “hours” then the PD payoffs have more influence on this player’s decision. In that case, α is small. Conversely, if α is large then the information about I is acquired frequently and the player acts accordingly. In this interpretation, the non-negative sign on α can be thought of as correctness in the player’s risk assessment. If the player thinks that a disease is dangerous and if the source of information is reliable, then the rational and conscious player acts with $\alpha \geq 0$.

3.3 Main results of Paper I

Paper I explores the steady state solutions to the combined SIS-PD and SIR-PD models. In the SIR-PD model at steady state, no one cooperates. This can probably be understood by the fact that the SIR model sees an end to the disease outbreak, so that once there is no spreading of disease there is also no will to cooperate. In the SIS-PD model, however, the balance parameter α plays a crucial role. The higher it is, the more individuals will cooperate, starting from 0% and going all the way to 100%. Since α can be interpreted as the perceived severity of having infected individuals in the population or the rate at which individuals receive information about the number of infectious people, this is a quite interesting observation.

3.3.1 SIS-PD equilibrium points

Recall that the SIS-PD model is defined by the set of equations (3.13)–(3.14) with $\beta_C < \beta_D$.

Theorem 3.1. *The equilibrium points of the SIS-PD system are*

$$(x, I) \in \left\{ (0, 0), (1, 0), \left(0, 1 - \frac{\gamma}{\beta_D}\right), \left(1, 1 - \frac{\gamma}{\beta_C}\right), (x^*, I^*) \right\}, \quad (3.15)$$

where

$$x^* = \frac{\beta_D}{\beta_D - \beta_C} - \frac{\gamma}{(\beta_D - \beta_C)(1 - I^*)}, \quad I^* = \frac{(C - N(k))}{\alpha(\beta_D - \beta_C)} \quad (3.16)$$

The equilibrium points are well-defined and stable under the conditions given in the following table.

Equilibrium	Condition
$(0, 0)$	$\beta_D < \gamma, \alpha(C - N(k)) > 0$
$(1, 0)$	$\beta_C < \gamma, \alpha(C - N(k)) < 0$
$(0, 1 - \gamma/\beta_D)$	$\beta_D > \gamma, \alpha \leq \check{\alpha}$
$(1, 1 - \gamma/\beta_C)$	$\beta_C > \gamma, \alpha \geq \hat{\alpha}$
(x^*, I^*)	$\hat{\alpha} < \alpha < \check{\alpha}, 0 < I^* < 1, 0 < x^* < 1$

Here,

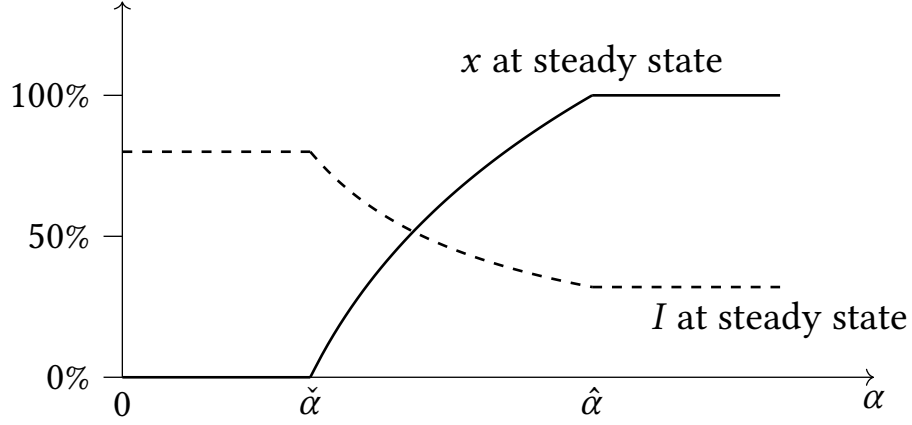
$$\check{\alpha} = \frac{\beta_D}{\beta_D - \gamma} \frac{C - N(k)}{\beta_D - \beta_C} \quad \text{and} \quad \hat{\alpha} = \frac{\beta_C}{\beta_C - \gamma} \frac{C - N(k)}{\beta_D - \beta_C}. \quad (3.17)$$

Since I denotes a portion we must have $0 \leq I \leq 1$ which is one main criterion for the steady states to be well-defined. The same holds for x . Proving the stability of each steady state solution also involves computing the Jacobian matrix of the SIS-PD equations. They are stable if the eigenvalues of the Jacobian matrix are negative [13].

Following the values of α , the equilibrium *transitions* between the asymptotically stable equilibrium points of Theorem 3.1. The following table shows the equilibria in three regions of α assuming $\gamma < \beta_C < \beta_D$. The transitions occur at $\check{\alpha}$ and $\hat{\alpha}$, which are defined in (3.17).

Range	Equilibrium
$\alpha \leq \check{\alpha}$	$(0, 1 - \gamma/\beta_D)$
$\check{\alpha} < \alpha < \hat{\alpha}$	(x^*, I^*)
$\hat{\alpha} \leq \alpha$	$(1, 1 - \gamma/\beta_C)$

The following figure is a visualization of the values in the above table.



As α increases, the population moves from defection ($x = 0$) to partial cooperation to cooperation ($x = 1$). At the same time, I , the portion of infectious individuals is decreasing. If α is sufficiently large and the transmission rate for cooperating individuals, β_C , decreases (still keeping $\gamma < \beta_C$) then the portion of infectious individuals tends to zero.

3.3.2 SIR-PD equilibrium points

Recall that the SIR-PD model is defined by the set of equations (3.9)–(3.12). Computing the Jacobian of this system, we identify the stable steady states precisely like in the above SIS-PD situation. Since $S + I + R = 1$, the quantity R at equilibrium is given by $R^* = 1 - S^*$ in the following theorem.

Theorem 3.2. *The SIR-PD model always stabilizes to a set of equilibrium points (x^*, I^*, S^*) with*

$$x^* \in \{0, 1\}, \quad I^* = 0, \quad 0 \leq S^* \leq 1. \quad (3.18)$$

All of these are possible; the exact values are determined by initial conditions. The equilibrium points with $x = 0$ are stable if $\beta_D S < \gamma$. If $\beta_D S > \gamma$ the equilibrium point is unstable. All equilibrium points with $x = 1$ are unstable.

Only the outcome with no cooperation whatsoever, $x^* = 0$, is stable in the SIR-PD model, which is actually expected because the SIR model “empties” the I -compartment. At steady state there are no infectious individuals left; the SIR model terminates at a no-disease state. Therefore, there is nothing to gain from cooperating. Looking at the dynamics before steady state,

however, there is an increase of cooperators during the outbreak of the disease.

3.3.3 What if we get used to the news?

Humans can get used to the current state (of knowledge, of financial status, etc.) and it is possible that *changes* are more important to peoples' choices than absolute values. It is therefore interesting to investigate what happens when the portion of “cooperating” individuals is dependent on the change of the infectious portion rather than the portion itself. In other words, what if $\dot{x}$ depends on $\dot{I}$ rather than I . Instead of the SIR model equations (3.10) and (3.12), consider

$$\dot{I} = ((1-x)\beta_D + x\beta_C)SI - \gamma I \quad (3.19)$$

$$\dot{x} = x(1-x)(\alpha(\beta_D - \beta_C)\dot{I} - (C - N(k))) \quad (3.20)$$

For the sake of simplicity, assume that $N(k) = 0$. It can be re-introduced later by changing C to $C - N(k)$. Then,

$$\begin{aligned} \dot{x} &= x(1-x)(\alpha(\beta_D - \beta_C)((1-x)\beta_D + x\beta_C)SI - \gamma I - C) \\ &= -x(1-x)x\alpha(\beta_D - \beta_C)^2SI + x(1-x)(\alpha\beta_D(\beta_D - \beta_C)SI - C) \\ &= x(1-x)(\alpha\beta_D(\beta_D - \beta_C)SI - C - x\alpha(\beta_D - \beta_C)^2SI). \end{aligned}$$

The stationary points are found by solving $\dot{x} = 0$ and $\dot{I} = 0$. By equations (3.19) and (3.20), that is equivalent to

$$0 = ((1-x)\beta_D + x\beta_C)SI - \gamma I \quad (3.21)$$

$$0 = x(1-x)C \quad (3.22)$$

By the latter of these, either $x = 0$, $x = 1$ or $C - N(k) = 0$ if we bring back $N(k)$ to the equations. The condition on $C - N(k)$ is, by the definition of the payoffs and the network correction $N(k)$, equivalent to

$$0 = T(k-1) - Rk.$$

In particular, for a well-mixed environment and Prisoner's dilemma payoffs, $T > R$, which leaves only the options $x = 0$ or $x = 1$. Recalling the

equation for R in the SIR model, $\dot{R} = \gamma I$, the stationary points are such that $I = 0$ which implies that Equation (3.21) is always satisfied. Moreover, $I = 0 \implies \dot{S} = 0$. By analyzing the perturbations away from the equilibria, it is concluded that $x^* = 0$ is an equilibrium if $I^* = 0$ is stable, which it is under the condition $\beta_D S^* < \gamma$. The equilibrium with $x^* = 1$ is never stable. To sum up, the results of Theorem 3.2 are recovered also when the population reacts to the rate of that of I .

In contrast to the SIR-PD model, the steady state for the SIS-PD model changes if the ratio of collaborators react to the rate of change of I . In this case, again,

$$\dot{x} = x(1-x)(\alpha(\beta_D - \beta_C)\dot{I} - (C - N(k))).$$

Therefore, at steady state when $\dot{I} = 0$, then x is either one or zero. The only stable equilibrium is $x^* = 0$, $I^* = 1 - \gamma/\beta_D$. The equilibrium at intermediate values of x , which could be observed in the SIS-PD model in Section 3.3.1, disappear under the assumption that the change of the number of infectious individuals determine the will to collaborate in the population.

4

The Game of Teams

They say: Winners and losers are two of a kind.

—Hamilton, Joe Frank & Reynolds (1976)

The Game of Teams has been developed during the last couple of years as a model to explain why certain compositions of team members are more advantageous than others. Central to this game is the assumption that competition occurs on an individual level whereas strategies are defined on a team-level. This applies in a wide range of situations such as economy (portfolio theory, management etc.), research, sports, behaviorological sciences and ecology. It has been demonstrated that diversity is beneficial in all these contexts. Results from ecology shows that diversity is healthy for a biological system, for instance as protection against extinction of species. Similarly, a diverse portfolio of investments protects the investor from financial backlash in case individual investments are unstable. Teams of scientists perform better if they are diverse in all senses they can be.

The game of teams do not treat teams as individuals and herein lies its importance. We construct a simple game in this chapter and we show that the success of a team depends heavily on the distribution of resources among its members. This provides an explanation to the strength of diversity without restricting the results to a specific context, such as ecology. The Game of Teams is developed to emphasize the difference between members in successful teams without the detailed knowledge of the underlying biological system (such as which food chains or geographic considerations

that would influence the fitness of individuals). Of course, this simplification can be questioned. As a professor in biology once told me at a poster session: “I think this is a situation when mathematicians think that the world is simpler than it really is.”

4.1 The evolution of the Game of Teams

This section introduces the *Game of Teams*, which was first defined by Menden-Deuer and Rowlett [54, 55] and later revised and refined in their follow-up collaborations [56]. Originally designed to explain the vast diversity among asexually reproducing (cloning) microbes and microbial subspecies, this game has a terminology of biology: The “players” are individuals and “teams” are species. We may also see terms such as population sizes and traits. In particular, the Game of Teams (or just the team game) identifies strategies in the game with traits.

In a well-mixed population, every member has a constant probability of meeting every other member. There are no closed groups but everyone has the same chance of meeting everyone. In a well-mixed population we may consider “teams” or “species” as labels and assign different characteristics to these teams. Imagine that two such teams constitute a population and that for each timestep the members of the population meet with a member from the other species and compare “strength”, meaning that

- if one member is stronger than the other, the stronger one defeats the weaker and then replicates, or
- if both members are equally strong, it is a draw and both players remain in the game.

A draw results in no change to the size of each team, but if a member of one team defeats a member from the other team there is an increase by one to the first team while the other team is reduced by one member. Imagine that these individual competitions take place simultaneously. If a member cannot be paired with another member, it waits until the rest of the members have compared strength. This is a timestep, or turn, in

the game of teams. To paraphrase a famous author [50], when you play the game of teams, you win or die or nothing happens. There is usually a middle ground.

Strength is here a positive, real number. An individual's strength is referred to as its *competitive ability*, in short CA. It should be assumed that the competing species, or teams, are on average not stronger than some positive number C . Otherwise it would be easy to win: just let all members of your team grow stronger. Thus, teams are characterized by the *distribution* of strength among the team members.

Example 4.1. Assume that two teams of three players each are playing cards with a special kind of deck: the cards can have five values 1, 2, 3, 4 or 5 and each team member can select one card as long as the average card value over the team is 3. Two or more players can select the same value. Each member pairs up with a member from the other team and the one having the highest value wins. What is the best strategy in this situation? Let A be one team and B be the other. If A always plays with the number 3 while B selects 4 for two of its members and 1 for the remaining member, which team is expected to win? In each turn, the number of players in A that are expected to win are the number of players in B that play 1 or 2 and those players in B playing 4 or 5 will always win. Let $n_B(x_j)$ be the number of members of B that play j . Then

$$n_B(x_1) + n_B(x_2) - n_B(x_4) - n_B(x_5) \quad (4.1)$$

is the increase of members to team A at each turn. This sum equals $1 + 0 - 2 - 0 = -1$ meaning that A wins one player but also loses two players; B wins the first turn. The teams are not equally strong even though their average strength is the same. Team B wins because it has a smarter distribution of competitive ability among its members.

Let N_B denote the number of individuals in B . Interpreting $n_B(x_j)/N_B$ as the probability that a random player in B has the strength x_j , we can say that n_B is a strategy. It is in fact the number of players in B that are expected to play x_j . The team A in this example plays with the strategy $n_A(x_3) = 3$ and $n_A(x_j) = 0$ for $j = 1, 2, 4, 5$.

We should think of strategies as assignment rules. At each turn, the strategy is the distribution of CA over the population in the sense that each player gets a CA randomly following the probability distribution given by the normalized strategy under the constraint that the average of the CAs is not greater than some number (which is 3 in the above example). Sometimes we do not distinguish a team from its strategy but rather we use strategy and team interchangeably. Next, some of the central mathematical notions are introduced in order to help answer the question about which team is the best.

4.1.1 Analytical tools and definitions

In the first publications on the Game of Teams, the strategy of a team A was defined to be non-negative numbers $n_A(x_i)$ for each fraction $x_i = i/M$ with $i = 0, 1, 2, \dots, M$ such that at least one of them is non-zero [55]. Here, M is a positive integer. Then the fractions range from 0 to 1. A strategy could look like in Figure 4.1. This one is symmetric about the midpoint value $1/2$.

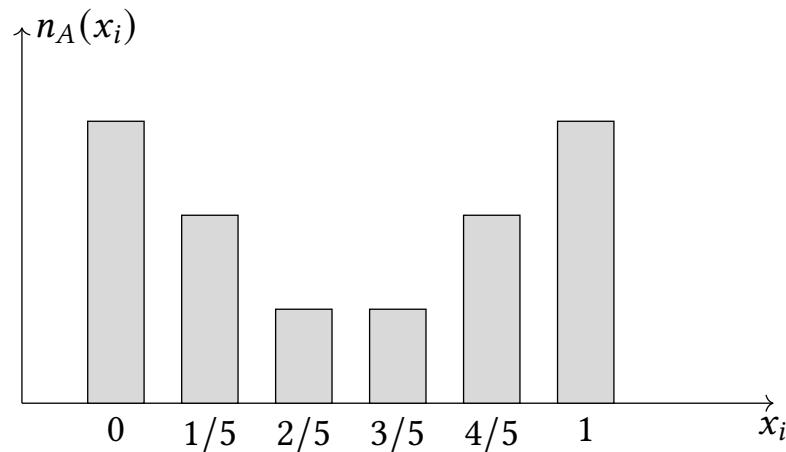


Figure 4.1: A strategy on the CAs $x_i = i/M$ for $M = 5$ and $i = 0, 1, 2, 3, 4, 5$.

As the theory evolved into a better, more general set of conclusions and results, these assumptions were removed and the fraction values were allowed to be many more than $M + 1$ and M did not need to be an integer. Thus, let M be a real, positive number and let a be an integer. Define for

all non-negative integers j the fractions

$$x_j = \frac{j + a}{M}. \quad (4.2)$$

It will be shown later that $a = 0$ without loss of generality. If we consider strategies from this set of x_j , we say that the game is the *discrete game of teams*. In this case we define strategies as follows.

Definition 4.1. Let A be a team. A *discrete strategy* of A is a mapping n_A from $\{x_j\}_{j \geq 0}$ into the non-negative, real numbers such that $n_A(x_j)$ is not identically zero and only finitely many $n_A(x_j)$ are non-zero.

In general in the discrete game, the species A expects a population increase (or decrease) in competition with B given by

$$E[n_A, n_B] = \frac{\min\{N_A, N_B\}}{N_A N_B} \sum_{i \geq 0} n_A(x_i) \left(\sum_{i > j} n_B(x_j) - \sum_{i < j} n_B(x_j) \right) \quad (4.3)$$

where an empty sum is interpreted as zero. The factor in front of the sums accounts for the situation that one team is smaller than the other. If, say, $N_A = 100$ and $N_B = 99$ then

$$E[n_A, n_B] = \sum_{i \geq 0} \frac{n_A(x_i)}{N_A} \left(\sum_{i > j} n_B(x_j) - \sum_{i < j} n_B(x_j) \right)$$

so then $E[n_A, n_B]$ is ranging from -99 to 99 , which is exactly the minimal and maximal number of “lose” and “win” that the team A could experience, since one member of A cannot be paired with a member of B . If we are interested in the relative increase, we compute $p[n_A, n_B] = E[n_A, n_B] / \min\{N_A, N_B\}$ or equivalently

$$p[n_A, n_B] = \sum_{i \geq 0} \frac{n_A(x_i)}{N_A} \left(\sum_{i > j} \frac{n_B(x_j)}{N_B} - \sum_{i < j} \frac{n_B(x_j)}{N_B} \right). \quad (4.4)$$

Game-theoretically, $p[n_A, n_B]$ is the payoff to team A in competition with B . The relative expectation, p , ranges from -1 to 1 . Passing between E and p simply means that we normalize the strategies. The expectation E and the payoff p satisfy the zero-sum property $E[n_A, n_B] + E[n_B, n_A] = 0$.

If more than two teams compete, every team experience competition from all the other teams. Let now f , g_1 and g_2 be three strategies according to Definition 4.1. Since the payoff p is a linear function of strategies,

$$p[f, g_1 + g_2] = p[f, g_1] + p[f, g_2], \quad (4.5)$$

we may define the expected payoff to f in competition with a collection of strategies $\{g_i\}_{i=1}^n$ as $p[f, g_1 + \dots + g_n]$. The linearity property (4.5) does not hold for E due to the factor α , but nevertheless we define the expectation of f in competition with a collection of species $\{g_i\}_{i=1}^n$ as $E[f, g_1 + \dots + g_n]$ since any species competes against all the others. The notation f is motivated by the function-valued game that is introduced below; it has the same definitions as here.

An *equilibrium* (or *equilibrium point*) in the game of teams is defined as a collection of strategies $\{f_i\}_{i=1}^n$ that satisfy the following condition: For each $k \in \{1, 2, \dots, n\}$, if team no. k changes its strategy but all other teams retain their strategies then the payoff to team no. k does not increase. This means that for all $k \in \{1, 2, \dots, n\}$,

$$p[f_k, f_1 + f_2 + \dots + f_{k-1} + f_{k+1} + \dots + f_n] \geq p[g, f_1 + f_2 + \dots + f_{k-1} + f_{k+1} + \dots + f_n]$$

for any strategy g of the same type as all f_i . The strategies that comprise an equilibrium point are known as *equilibrium strategies*.

One further defines the *non-exploitable* strategies [55] as those strategies f that satisfy $E[f, g] \geq 0$ for all strategies g . In other words, a non-exploitable strategy never loses. One remark can be made about the definition of E . It is never important to retain the pre-factor $\min\{N_f, N_g\}/N_f N_g$ in its definition and neither is it important to normalize the strategies, since any equation on the form $E[f, g] \geq 0$ is equivalent to $p[f, g] \geq 0$.

A team could always get better if all members would be stronger, that is, if the CAs of the members were allowed to grow without any constraint it would be trivial to construct a winning team. Assume therefore that only teams with an average CA of less than or equal to some positive number C are allowed to compete. We will refer to this as the constraint on the

mean competitive ability, or MCA, and we define

$$\text{MCA}(n_A) = \frac{\sum_{k \geq 0} x_k n_A(x_k)}{\sum_{k \geq 0} n_A(x_k)} \quad (4.6)$$

in the discrete game for a team A . It is usually assumed that $\text{MCA}(n_A) \leq \frac{1}{2}$ for all teams, but there are interesting results that deserve to be presented with a more general constraint $\text{MCA}(n_A) \leq C$ in some cases.

In nature, resources are limited and advantageous phenotypes usually come at a cost for the organism. If an organism gains the ability to resist, say, certain chemicals then it might sacrifice growth rate or efficiency in reproduction [39]. The MCA constraint reflects this need for compromise in nature.

4.1.2 The linear algebra formulation

In the discrete Game of Teams, the CA values (4.2) are set. In other words, they create the playground and shall not change even if it might be tempting to re-define the set of CAs. One implication of this is that strategies are equally well represented by vectors with non-negative components in the Euclidean space. The standard interval for the competitive abilities (4.2) is the unit interval, which amounts to choosing $a = 0$ and $j = 0, 1, 2, \dots, M$. Then, a discrete strategy (Definition 4.1) can be thought of as a vector-valued map f from $\mathbb{R}^{M+1}$ into $\mathbb{R}^{M+1}$. Define the matrices

$$f = \begin{bmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_M) \end{bmatrix}, \quad L = \begin{bmatrix} 0 & -1 & -1 & \dots & -1 \\ 1 & 0 & -1 & \dots & -1 \\ 1 & 1 & 0 & \dots & -1 \\ \vdots & & & & \\ 1 & 1 & 1 & \dots & 0 \end{bmatrix}, \quad (4.7)$$

where L is a square matrix of size $(M+1) \times (M+1)$. Then the payoff to a strategy f_1 in competition against f_2 is

$$p[f_1, f_2] = f_1 \cdot L f_2, \quad (4.8)$$

where $f_1 \cdot L f_2 = f_1^\top L f_2$. Here, f_1 and f_2 are suitably normalized.

4.1.3 Function-valued games

If the CAs that are available to the teams are *many*, it seems like a discrete strategy could approximate a function. Indeed, the payoff (4.4) would be a Riemann sum that converges to integrals as $M \rightarrow \infty$ (if the strategies are bounded). Conversely, it is possible to think about the discrete strategies as *samples* of a function-valued strategy. Let f be a function and let $f(x_i)$ be its value at the CA with label i . Then $n_A(x_i) = f(x_i)$ defines a discrete strategy. This motivates the following definition.

Definition 4.2. A *bounded strategy* is a Lebesgue-measurable, bounded, non-negative function $f : [0, 1] \rightarrow \mathbb{R}$ that is not identically zero.

If the strategies are as in Definition 4.2, we call this the *bounded game of teams* or the *bounded measurable game of teams*. We refer to the *continuous game of teams* if in addition to the requirements in Definition 4.2 it is required that strategies are continuous functions.

There is a probabilistic way to think about the function-valued strategies. If a continuous strategy f is given and is such that $\int_0^1 f(x) dx = 1$ then the integrals

$$\int_a^b f(x) dx$$

over intervals (a, b) are the probabilities that an individual's CA is in the range between a and b . This is the gray area in Figure 4.2. To be able to define these probabilities, the functions could be unbounded. It would be fine to work with functions of class L^1 , since the interpretation of samples in this case would be the integral over an interval. In this class, a strategy can be defined as a Lebesgue-measurable, non-negative function $f \in L^1[0, 1]$ such that $\int_0^1 f(x) dx > 0$. If $\int_0^1 f(x) dx = 1$, these functions are representing probability density functions of the CAs.¹

¹Notice that if an integrable real random variable X has a distribution P_X with density f with respect to the Lebesgue measure, then the expectation of X is the MCA of f . This expectation is not related to the expectation in competition as defined in this chapter.

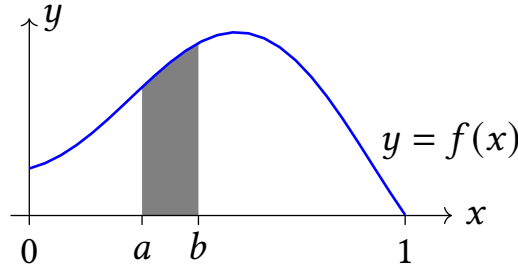


Figure 4.2: Function-valued strategies can be thought of as distribution of competitive ability. If the function is normalized then the integral over the interval (a, b) is the percentage of individuals with competitive ability between a and b .

Since the functions of interest are closely related to the L^p spaces L^1 and L^∞ , it is also motivated to study the general L^p spaces for any integer $p \geq 1$. This is central to Paper IV.

For function-valued strategies, we define the expectation of a strategy f in competition with another strategy g as

$$E[f, g] = \alpha \int_0^1 f(x) \left(\int_0^x g(y) dy - \int_x^1 g(y) dy \right) dx \quad (4.9)$$

where α is the prefactor

$$\alpha = \frac{\min \left\{ \int_0^1 f(x) dx, \int_0^1 g(x) dx \right\}}{\left(\int_0^1 f(x) dx \right) \left(\int_0^1 g(x) dx \right)}. \quad (4.10)$$

Again we define p as $p[f, g] = E[f/F, g/G]$ where F and G are the integrals of f and g over $[0, 1]$, that is, we normalize them with respect to the L^1 norm. Integration here means integration with respect to Lebesgue measure. Both E and p satisfy the zero-sum property

$$p[f, g] + p[g, f] = 0 \quad (4.11)$$

in the bounded, the continuous and the discrete game.

In Paper II, we use the notation $\wp$ (this symbol is called the “Weierstrass p ”) for the expectation E with $\alpha = 1$. We also use the notation $\wp[f; g_1, \dots, g_n] =$

$\wp[f, g_1 + \dots + g_n]$. Again, using E or $\wp$ does not change which strategies are equilibrium strategies, so we may use $\wp$ instead of p .

In the bounded game as well as in the continuous game we define the mean competitive ability of a team with strategy f to be

$$\text{MCA}(f) = \frac{1}{\int_0^1 f(x) dx} \int_0^1 x f(x) dx. \quad (4.12)$$

The game is invariant to scaling and translating the unit interval, see Section 4.2, which implies that the above definitions are readily made for functions on any interval $[a, b]$ for $a < b$. In Paper II, we assume that the strategies are defined on $\mathbb{R}$ with support on some compact subset of $[x_0, \infty)$ for some real number x_0 . This number, x_0 , is the same for all strategies in a competition. The equivalent of $\int_0^1 f(x) dx$ is then $\int_{x_0}^{\infty} f(x) dx$ and so on. That is, all integrals are taken over the real line $\mathbb{R}$.

4.1.4 Adaptive dynamics

In the game of teams, as traits are described by a distribution of strength, we think of a mutation as a sudden change to the shape of the distribution, see figure 4.3. The mutation process is assumed to be separated from the natural selection; the spread of a mutation *within* a species is assumed to be instantaneous compared to the timescale of the evolutionary game *between* species [57, 25, 7]. In other words, if a mutant has lower fitness than the resident population then it disappears, but if the mutant's fitness is higher than the resident population's then it is assumed that the mutation spreads into the entire resident population. This leads to a so-called trait exchange, leaving the entire population with the new trait. Referring to figure 4.3, if the subpopulation of mutated individuals having the slightly altered distribution (the blue line) perform better in competition against the resident population (the black line), then the evolution proceeds in the direction of the mutation.

As the game of teams is not only defined for discrete strategies but also for strategies that are functions, we consider the adaptive dynamics framework by Dieckmann, Heino and Parvinen [15]. In addition to the application of

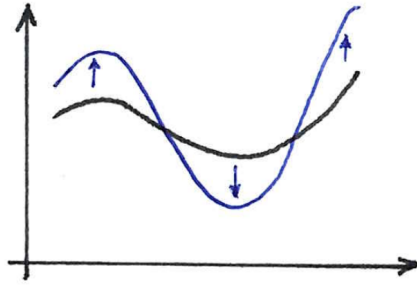


Figure 4.3: Mutations in the team game alters the strategy of the “resident” population and introduces a new “mutant” distribution.

their theory, the intent of Paper IV was to subject adaptive dynamics to a more rigorous mathematical treatment.

Since the expectation $E[f, g]$ in the team game is interpreted as the expected growth rate of f in competition with g , it also defines the invasion fitness of a mutant in a resident population. Following the presentation of Chapter 2, the initial growth rate of the mutant subpopulation is given by the formula

$$\nabla E(f)(x) = \left. \frac{d}{dt} \right|_{t=0} E[f + t\delta_x, f]. \quad (4.13)$$

The map ∇E takes a strategy f and returns a function called the selection gradient. It defines the *direction of change* of the resident population’s traits via the canonical equation of function-valued traits, Equation (2.22). From the definition of E in (4.9), ignoring the pre-factor, it follows that

$$\nabla E(f)(x) = \int_0^x f(y) dy - \int_x^1 f(y) dy. \quad (4.14)$$

In order to complete the description of the evolution of traits, the variance-covariance function of Equation (2.22) has to be specified. In particular, the MCA constraint $\text{MCA}(f) \leq \frac{1}{2}$ is encoded into σ_f^2 . One would like to generalize this to constraints on the form $w(f) = 0$ for some w mapping from the set of strategies to the real numbers.

Since Paper IV explains how $w(f) \leq 0$ is incorporated in the dynamics on the function-valued strategies, let us do it for the vector-valued strategies here. Let f be a vector as in Section 4.1.2. The constraint $\text{MCA}(f) \leq \frac{1}{2}$

can be expressed as

$$w(f) \leq 0 \quad \text{for} \quad w(f) = \sum_{k=0}^M (x_k - \frac{1}{2})f(x_k) \quad (4.15)$$

The projection onto the tangent of the boundary $w(f) = 0$ is the vector $P(f)$ with components

$$P_j(f) = \frac{\langle f, \nabla w \rangle}{\|\nabla w\|^2} (x_j - C).$$

Here, $\langle , \rangle$ is the ℓ^2 inner product

$$\langle f, g \rangle = f^\top g = \sum_{k=0}^M f(x_k)g(x_k)$$

and $\|\nabla w\|^2 = \langle \nabla w, \nabla w \rangle$. The idea is that $I - P$ maps a strategy into the regime of MCA equal to $\frac{1}{2}$, so if a strategy increases its MCA, then it will do so until its MCA equals $\frac{1}{2}$ and then $I - P$ is applied to the selection gradient to ensure that the MCA does not increase further. This ensures that the constraint in (4.15) is respected at all times.

The resulting adaptive dynamics of the team game can be described by a time-dependent strategy f and the evolution equation

$$\frac{d}{dt}f = Af \quad (4.16)$$

where $A = L$ whenever $\text{MCA}(f) < \frac{1}{2}$ and $A = (I - P)L$ whenever $\text{MCA}(f) \geq \frac{1}{2}$. With an initial value on the strategy, f_0 , that is a “current” strategy at time $t = 0$, this is an initial value problem. The strategies and the mapping A will have the same meaning in the vector-valued game as in the function-valued game. For the function-valued game, define the right hand side of the adaptive dynamics equation (4.16) to be the function Af given by

$$\begin{aligned} Af(x) = & \int_0^x f(y) dy - \int_x^1 f(y) dy \\ & - 12H(w(f))(x - \frac{1}{2}) \int_0^1 \left(y - \frac{1}{2}\right) \left(\int_0^y f(z) dz - \int_y^1 f(z) dz\right) dy. \end{aligned} \quad (4.17)$$

This is simplified using the notation for the projection P and the definition of the selection gradient:

$$Af(x) = (I - H(w(f))P)\nabla E(f). \quad (4.18)$$

In the discrete game, the selection gradient is Lf , where f is a vector of strategy values at each CA. Then

$$Af = (I - H(w(f))P)Lf. \quad (4.19)$$

Notice that the Heaviside function introduces a non-linearity.

4.2 Main results of Paper II

It might seem like, at this point, the game has been restricted a lot due to the assumption that the strategies are supported on $[0, 1]$ and that the MCA constraint is $\text{MCA}(f) \leq \frac{1}{2}$. However, the game of teams is *translation invariant* and *scale invariant*. This means that given a collection of strategies we may assume that they are defined on $[0, 1]$ or some other interval, say $[-1, 1]$. If f and g are two strategies, their support is contained in a closed interval $[a, b]$ such that $a < C < b$. Defining $\ell = b - a$, $\tilde{C} = (C - a)/\ell$ and

$$\tilde{f}(t) = \ell f(\ell t + a), \quad \tilde{g}(t) = \ell g(\ell t + a) \quad \text{for } t \in [0, 1] \quad (4.20)$$

we have

$$\begin{aligned} \text{MCA}(f) \leq C &\iff \text{MCA}(\tilde{f}) \leq \tilde{C}, \\ \text{MCA}(g) \leq C &\iff \text{MCA}(\tilde{g}) \leq \tilde{C} \end{aligned}$$

and $p[\tilde{f}, \tilde{g}] > 0 \iff p[f, g] > 0$. This implies that the value of E and p are unchanged under the translations

$$x \mapsto x + x_0, \quad C \mapsto C + x_0, \quad (4.21)$$

with $x_0 \in \mathbb{R}$ in the bounded or continuous game, and correspondingly for the discrete game $j \mapsto j + a$, $C \mapsto C + x_a$ with $a \in \mathbb{Z}$. Therefore, if the

strategies are defined on a compact subset of $[x_0, \infty)$ for some x_0 , one may assume that $x_0 = 0$. If the strategies are supported in $[a, b]$ then they are also supported in $[a, b']$ for some $b' > b$, so it is possible to assume that $C \leq \frac{1}{2}(b-a)$. In other words, it is only the distance to C that matters for the outcome of the game and assuming $C = \frac{1}{2}$ is not a very strict assumption.

One may of course ask whether it is necessary to have a lower bound at all on the CAs. The answer is: Yes, that is, if we want the game to be interesting, because if there is no lower bound on the CAs then we may always construct a species similar to the winning species in Example 4.1 and easily win. That is, any team could win in that case, just by sending one player to very low CAs and assign to the rest of its members a CA which is just slightly higher than those of the competing species' CAs. A winning team is trivial to construct if the CAs are not bounded from below.

The definition of non-exploitable strategies agrees with the definition of a Nash equilibrium. By the following proposition, it is equivalent to non-negative expectation in competition with any other strategy. A proof of this proposition is found in Paper II.

Proposition 4.1. *Assume that a collection of strategies $\{f_i\}_{i=1}^n$ is an equilibrium point. Then they satisfy*

$$p[f_j, f_k] = 0 \text{ for all } k, j, \quad \text{and} \quad p[f_k, g] \geq 0 \text{ for any strategy } g. \quad (4.22)$$

Equivalently, each f_k is an equilibrium strategy for the two-player game. Conversely, if $\{f_i\}_{i=1}^n$ satisfy (4.22) then $\{f_i\}_{i=1}^n$ is an equilibrium of the game.

4.2.1 Equilibrium strategies

In Paper II we identified the equilibria for the game of teams. In the bounded game of teams, a strategy is an equilibrium strategy if and only if it is almost everywhere equal to, for some constant $K > 0$,

$$f(x) = \begin{cases} K, & x \in [x_0, 2C - x_0] \\ 0, & \text{otherwise.} \end{cases} \quad (4.23)$$

This is a constant, positive function with support on an interval centered around C . There are no equilibrium strategies in the continuous game of teams, because it would need to equal (4.23) which is not continuous.

Remark. Considering the continuous game, it is important to pay attention to the definition. If the functions are defined on any compact support on $[0, \infty)$ as in Paper II, then there are no continuous Nash equilibrium strategies. In Paper IV, the functions are defined on $[0, 1]$ and then the Nash equilibrium point in the function-valued game consists of constant functions on $[0, 1]$.

Corollary 3.7 of Paper II, says that if $\text{MCA}(f) \leq \frac{1}{2}$ for all function-valued strategies, all equilibrium strategies in the bounded measurable game of teams for functions supported in $[0, 1]$ are positive constants on the unit interval, and conversely, all equilibrium points comprise positive constant functions. In the continuous game of teams restricted to a fixed interval $[a, b]$ with constraint value $C = (b + a)/2$ all equilibrium strategies are positive constant functions on $[a, b]$.

Recall the definition of the fractions x_j in (4.2). In the discrete game, assume that the MCA-constraint is such that C lies on some CA or precisely between CAs, that is,

$$C = \frac{a + \frac{1}{2}k}{M} \quad \text{for some integer } k > 0. \quad (4.24)$$

A team A has an equilibrium strategy n_A if and only if it is given by a constant $b > 0$ and if k is odd,

$$n_A(x_j) = \begin{cases} b, & 0 \leq j \leq k \\ 0, & \text{otherwise} \end{cases} \quad (4.25)$$

or if k is even, for a and b non-negative constants that are not both zero (and where a is *not* necessarily the same constant as in the definition of C),

$$n_A(x_j) = \begin{cases} a, & 0 \leq j \leq k, j \text{ even} \\ b, & 1 \leq j \leq k - 1, j \text{ odd} \\ 0, & \text{otherwise} \end{cases} \quad (4.26)$$

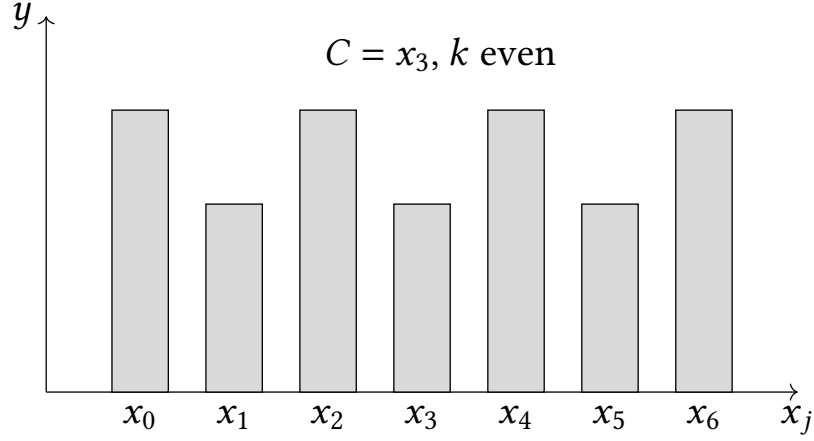


Figure 4.4: A Nash equilibrium in the discrete game with k even.

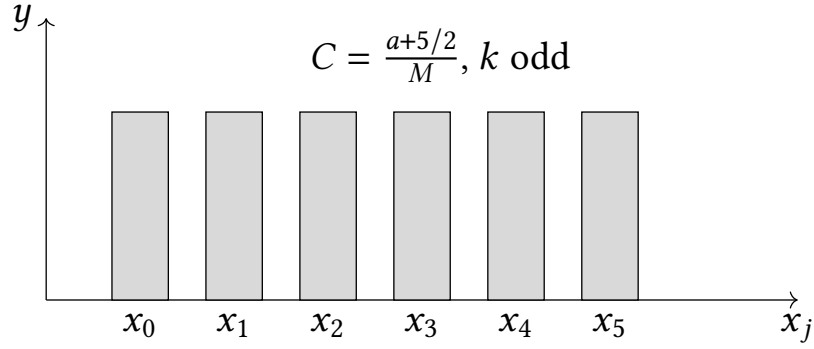


Figure 4.5: A Nash equilibrium in the discrete game with k even.

In (4.26), not all n_A 's are zero by definition of a strategy but either a or b can be zero. Conversely, when there exists an equilibrium in the game of teams, it is comprised of the above strategies. A visualization of these equilibrium strategies are provided in Figure 4.4 and Figure 4.5.

Figure 4.6 is a visualization of the equilibrium strategies of the bounded game with $x_0 = 0$, which is no limitation due to translation invariance. Notice that this is a discontinuous function. In fact, this is the reason that there are no equilibrium strategies in the continuous game of teams. Any continuous function will lose against a continuous function that better mimics the equilibrium of the bounded game, but then no function will ever be protected against losing the game, so there is no equilibrium. As already remarked, if the game would be defined on $[0, 1]$ for functions with $\text{MCA}(f) \leq \frac{1}{2}$ rather than any compact subset of $[x_0, \infty)$, then the

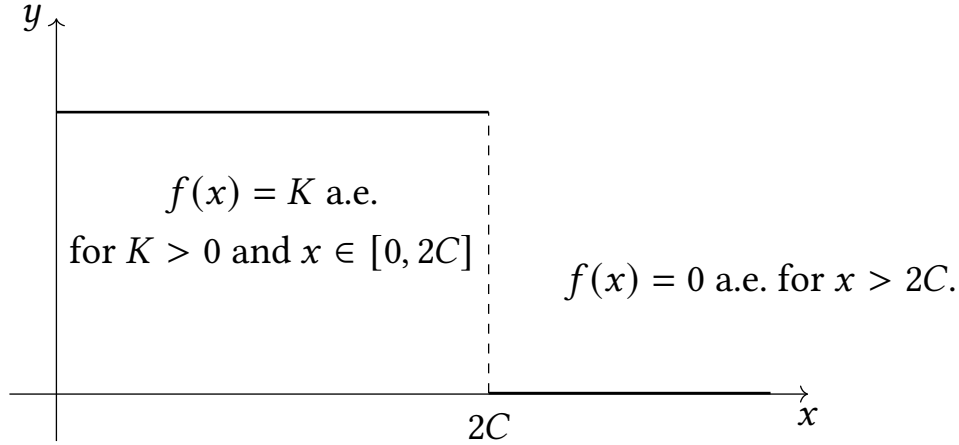


Figure 4.6: The unique Nash equilibrium in the bounded game.

constant functions on $[0, 1]$ are equilibrium strategies.

Proving these results requires computing the expectation between pairs of strategies and using Proposition 4.1. In the bounded game we show that $E[f, g] \geq 0$ for f given by (4.23) and any other strategy g by direct computation of E . As mentioned above, given any collection of strategies one can assume that they are defined on the interval $[0, 1]$ with $C \leq 1/2$ by the change of variables in (4.20). Then the continuous strategies and the discrete strategies satisfy the conditions of Theorem 1 in [56]. These are some of the main arguments that prove the results of Paper II.

Equilibrium strategies are positive and constant on an interval centered around C . In Paper II we note that such functions distribute the CAs without favoring any values in particular. Every CA is equally probable, so the teams will have “maximal distribution” of team members and all members are treated equally. This motivates the title of the paper, *Diversity strengthens competing teams*.

How well does an equilibrium strategy perform? Even if it is, in the sense of Nash equilibria, the best strategy, it does not win against every other strategy. In fact, what makes it an equilibrium strategy is the fact that it never loses. Consider the non-negative, measurable functions on the unit interval $[0, 1]$. A quick calculation shows that

$$E[u, g] = \frac{\min\{N_u, N_B\}}{N_u N_g} \left(\frac{1}{2} - \text{MCA}(g) \right) \quad (4.27)$$

where u is a constant function (the *uniform* distribution). That is, *all* functions that satisfy $\text{MCA}(g) = \frac{1}{2}$ will co-exist with u . The Nash equilibrium has infinitely many friends!

One bit of critique of the wording “strength” has been proposed to me. Let u be a constant function. If the CA is a resource such as money, then the “richest one percent” will have $\int_{1-0.01}^1 x u(x) dx = 9.9\%$ of the resources, which is a lot compared to the other end of the spectrum: The “poorest one percent” has only $\int_0^{0.01} x u(x) dx = 0.005\%$ of the resources. The Nash equilibrium is very unfair.

4.3 Main results of Paper IV

Paper IV formalizes the adaptive dynamics framework and applies it to the team game. The evolution of the game’s strategies are described both for the discrete game and for the function-valued game. One major result is the agreement between stationary points and the Nash equilibria.

Many of the results in Paper IV derive properties of the adaptive dynamics map A defined in §4.1.4. This mapping can be written on the form $A = (I - P)L$, where these components of A are matrices for the vector-valued game while they are integral operators in the function-valued game. The projection P applies to strategies with MCA equal to $\frac{1}{2}$, while it is removed if their MCA is less than $\frac{1}{2}$. The map A takes a strategy and maps it to the derivative of the strategy with respect to time: $\mathbf{y}'(t) = A\mathbf{y}(t)$. Therefore, if a strategy $\mathbf{y}$ is such that $A\mathbf{y} = 0$ then it is a stationary solution. It might seem like a complicated manner to solve $A\mathbf{y} = 0$ by considering the more general eigenvalue problem $A\mathbf{y} = \lambda\mathbf{y}$, but it turned out that we could derive some results for both $\lambda = 0$ and some of the non-zero eigenvalues whenever they exist.

The mapping properties of A acting on functions are important to ensure that the problems are well-defined. Paper IV shows that A maps from $L^p[0, 1]$ into $L^p[0, 1]$ for any $p \geq 1$, including $p = \infty$. Moreover, $A :$

$L^p[0, 1] \rightarrow L^p[0, 1]$ is bounded and

$$\begin{aligned} A : L^p[0, 1] &\rightarrow W^{1,p}[0, 1], & 1 \leq p \leq \infty, \\ A : C^k[0, 1] &\rightarrow C^{k+1}[0, 1], & 1 \leq k < \infty. \end{aligned}$$

For the discrete game, we prove the following eigenvalue property of the matrix A .

Proposition 4.2. *For both $A = L$ and $A = (I - P)L$, the eigenvalue problem $A\mathbf{y} = \lambda\mathbf{y}$ is solved either by $\lambda = 0$ or $\lambda = \pm i\beta$ for some non-zero, real β .*

The algebraic multiplicities are unknown, except in case one considers strategies such that $\text{MCA}(\mathbf{y}) < \frac{1}{2}$. Then $A = L$. Let L be of size $(M + 1) \times (M + 1)$. The eigenvalue problem $L\mathbf{y} = \lambda\mathbf{y}$ admits $\lambda = 0$ with algebraic and geometric multiplicity one if $M + 1$ is odd. The reason why we know this is that we derived the characteristic polynomial of L . It is expressed in terms of binomial coefficients:

$$\det(L - \lambda I) = \sum_{k=0}^{(M+1)/2} \binom{M+1}{2k} \lambda^{2k}$$

whenever $M + 1$ is even, or if $M + 1$ is odd,

$$\det(L - \lambda I) = -\lambda \sum_{k=0}^{M/2} \binom{M+1}{2k+1} \lambda^{2k}.$$

The most important question is which strategies that are stationary, that is, on which strategies the adaptive dynamics do not impose evolution. In case $\text{MCA}(\mathbf{y}) < \frac{1}{2}$ is assumed, so that $A = L$, and the size of L is even, the above characteristic polynomial reveals that there are no stationary solutions at all. The matrix is full-rank. If the size of L is odd, however, then $\lambda = 0$ with algebraic multiplicity one, and its eigenspace is spanned by

$$(1, -1, 1, -1, \dots, 1, -1, 1). \quad (4.28)$$

The dynamics $\mathbf{y}' = L\mathbf{y}$ has only one stationary solution, namely the vector in (4.28). Since it will never have only non-negative components, it is not

a strategy, but still a stationary solution. For the case $\text{MCA}(\mathbf{y}) = \frac{1}{2}$, when $A = (I - P)L$, the geometric multiplicities are

$$\dim \text{Ker } (I - P)L = \begin{cases} 2, & M + 1 \text{ odd} \\ 1, & M + 1 \text{ even.} \end{cases}$$

Moreover, the vectors that span this eigenspace were determined, meaning that a basis for the stationary solutions could be obtained. The next theorem provides the details.

Theorem 4.3. *The only stationary solutions to the initial value problem $\mathbf{y}'(t) = A\mathbf{y}(t)$, $\mathbf{y}(0) = \mathbf{y}_0$, $A = (I - P)L$, are in each case: If $M + 1$ is even,*

$$\mathbf{y} = (1, 1, 1, \dots, 1)$$

or any constant times this $\mathbf{y}$. If $M + 1$ is odd,

$$\mathbf{y} = (1, 0, 1, 0, \dots, 0, 1) \quad \text{or} \quad \mathbf{y} = (0, 1, 0, 1, \dots, 1, 0)$$

or any linear combination of these. If $A = L$, the only stationary solution is (4.28) or any constant times this vector.

The stationary solutions for $A = (I - P)L$ have good properties in the context of the team game. Linear combinations of the stationary solutions with non-negative coefficients fulfil the criteria to define strategies: The components are non-negative and $\text{MCA}(\mathbf{y}) = \frac{1}{2}$.

The most important implication of the above theorem is that for discrete strategies, the stationary solutions are precisely the Nash equilibria. Indeed, the Nash equilibria for the discrete game in Section 4.2.1 are linear combinations of the stationary solutions of the above theorem. The converse statement is to say that whenever the initial data $\mathbf{y}_0$ is a stationary solution *and* is a strategy, then it is a Nash equilibrium. There are stationary solutions to the initial value problem that have negative components, for instance $\mathbf{y} = (-1, -1, -1, \dots, -1)$, which is not a strategy due to the condition that strategies have non-negative components.

If $\text{MCA}(\mathbf{y}_0) < \frac{1}{2}$, then the dynamics is determined by $A = L$. To the problem $\dot{\mathbf{y}} = A\mathbf{y}$ with $\mathbf{y}(0) = \mathbf{y}_0$, there is a stationary solution on the

form (4.28) if M is even, but it does not satisfy $\text{MCA}(\mathbf{y}_0) < \frac{1}{2}$. Instead, its MCA equals a half. Moreover, its components have opposite signs.

A number of other results were found, for instance that for strategies such that $\text{MCA}(\mathbf{y}) = \frac{1}{2}$, the sum of the components

$$\sum_{i=0}^M y_i$$

is constant as a function of time. This implies that a normalized strategy with $\text{MCA}(\mathbf{y}) = \frac{1}{2}$ can be interpreted as a probability density over the CAs. That is, it is a mixed strategy for all $t > 0$.

For the function-valued game, the adaptive dynamics equation (4.29) is better written in terms of a curve $\alpha : I \rightarrow L^p[0, 1]$, where I is an interval on the real line containing zero. For each t in this interval, $\alpha(t)$ is a function of L^p class. Assume that f_0 is a fixed element in $L^p[0, 1]$. Then α is the integral curve of A starting at f_0 if

$$\frac{d}{dt}\alpha(t) = A(\alpha(t)) \quad \text{with} \quad \alpha(0) = f_0. \quad (4.29)$$

It is showed in Paper IV that there is an integral curve to each initial data.

Theorem 4.4. *Let $p \geq 1$. Let A be as in (4.17) and $f_0 \in L^p[0, 1]$. Then the initial value problem (4.29) admits a solution $\alpha : [0, \infty) \rightarrow L^p[0, 1]$, which is C^1 -smooth, except at t if $w(\alpha(t)) = 0$ and $w(\alpha(t')) < 0$ for all $t' < t$ (there is one or no such t). If $f_0 \in C^k([0, 1])$ then the solution is also C^k at every time. If in addition $\int_0^1 f_0(x) dx \neq 0$ and $\text{MCA}(f_0) = \frac{1}{2}$ then $\text{MCA}(\alpha(t)) = \frac{1}{2}$ for all $t > 0$. If furthermore $f_0 \in L^p[0, 1]$ with $p \geq 2$ and $\text{MCA}(f_0) = \frac{1}{2}$ then the L^2 norm of the solution is constant with respect to time.*

This theorem is proved using Lemma 3.7 of Paper IV and the Picard-Lindelöf theorem for the cases $w(f) < 0$ and $w(f) \geq 0$. Introduce the notation $\alpha_t = \alpha(t)$ and $H(f) = H_f$ in order to avoid excessive use of parentheses. Lemma 3.7 shows that a solution α_t for the adaptive dynamics equation is such that $w(\alpha_t)$ is a strictly increasing function of t , were it not for the Heaviside function H in the definition of A . Precisely,

$$\frac{d}{dt}w(\alpha_t) = (1 - H_{w(\alpha_t)}) \int_0^1 (x - x^2) \alpha_t(x) dx. \quad (4.30)$$

The integral on the right hand side of (4.30) is positive if $\alpha_t(x) \geq 0$ and $\int_0^1 \alpha_t(x) dx > 0$, and $1 - H_{w(\alpha_t)} = 1$ if $0 < \text{MCA}(\alpha_t) < \frac{1}{2}$. The Heaviside function activates the projection map P . Thus, the solution transitions from $w(\alpha_t) < 0$ to $w(\alpha_t) = 0$ at some t and then stays at $w(\alpha_t) = 0$.

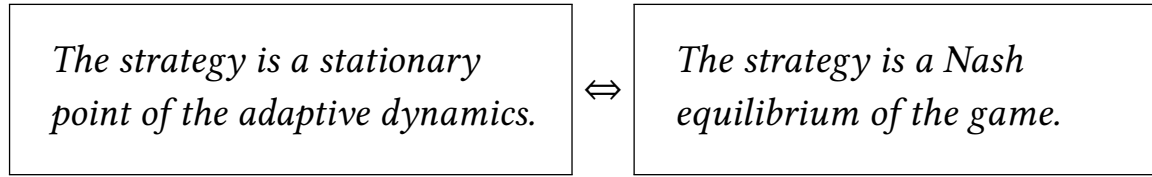
The continuity of the dynamics ensures that the solutions do not suddenly deviate from the initial condition. For functions in $L^\infty[0, 1]$, this ensures that initial strategies that are positive stay positive at least for some (possibly short) time.

Theorem 4.5. *Consider function-valued strategies in the bounded game. Let A be as in (4.17) and f_0 a bounded strategy such that $f_0(x) > 0$ for all $x \in [0, 1]$. Then the initial value problem (4.29) admits a solution α , which is C^1 -smooth as a function of time, except at t if $\text{MCA}(\alpha(t)) = \frac{1}{2}$ and $\text{MCA}(\alpha(t')) < \frac{1}{2}$ for all $t' < t$ (there is one or no such t). If $f_0 \in C^k([0, 1])$ then the solution is also C^k at every time. If in addition $\text{MCA}(f_0) = \frac{1}{2}$ then $\text{MCA}(\alpha(t)) = \frac{1}{2}$ for all $t > 0$ and the L^2 norm of the solution is constant with respect to time. The maximal time T is either $T = \infty$ or it is the largest time for which $\alpha(t)$ is a positive function on $[0, 1]$.*

Remark. The solution α in Theorem 4.5 is possibly satisfying the MCA constraint with strict inequality, $\text{MCA}(\alpha(t)) < \frac{1}{2}$, for all $t \leq T$. This is because the positivity condition could be broken before the MCA grows to $\frac{1}{2}$. However, if that is not the case, then (4.30) implies that the MCA grows until $\text{MCA}(\alpha_t) = \frac{1}{2}$ and then it stays at $\frac{1}{2}$.

Collecting the results both for the discrete (vector-valued) game and the function-valued game, it can be concluded that there is a correspondence between the Nash equilibria and the stationary solutions of the dynamics. This applies in the space of strategies and in particular, the values of the strategies at any CA are non-negative. Then we obtain the following powerful statement:

Theorem 4.6. *Consider a strategy in the team game and the evolution of strategies which is outlined in the above. Then:*



Remark. The statements in this equivalence theorem starts with “the strategy”. This is to emphasize that stationary points are Nash equilibrium strategies assuming that they are strategies to begin with. As already remarked, there are stationary solutions that are not strategies.

Remark. The definition of a function-valued strategy contains that the strategy is defined on the unit interval $[0, 1]$ and again, this means that both the bounded game and the continuous game admit a Nash equilibrium of constant functions. If instead the functions are defined on any compact support on $[0, \infty)$ as in Paper II, then there are no continuous Nash equilibrium strategies. It has not been investigated how the adaptive dynamics would evolve such functions. The selection gradient would probably need to be restricted to some compact support, which implies that there is a need for modeling choices, since there is no standard compact support for all functions.

While Theorem 4.6 connects the game theoretical optimality with the dynamic optimality, it does not reveal anything about the stability of the dynamics. In particular, it does not say whether the stationary point of the adaptive dynamics is convergence stable or connected. Of course, the linearity of the team game implies that the adaptive dynamics classification by Geritz *et al.* [25] does not apply, even if the phenomenological classification does, since their criteria are based on the convexity of the fitness function in a neighborhood of the stationary points.

All the real parts of the eigenvalues in the discrete game (for the cases $w(\mathbf{y}) < 0$ and $w(\mathbf{y}) \geq 0$, respectively) are zero, which means that the dynamics never shrinks exponentially to zero as time $t \rightarrow \infty$. In other words, the evolution continues indefinitely for any strategy that is not a stationary point. Biologically, this is reasonable in a model that claims to reflect any type of realistic evolution, since the evolutionary process by random mutations never ceases. Even species that appear to be “living

fossils” and look almost the same as they did millions of years ago have been and are still evolving [80].

One mathematical question which was left open for future researchers was the question about boundedness of the solutions. In every example of the discrete game with $\text{MCA}(\mathbf{y}) = \frac{1}{2}$, we observed that there are no polynomials (of order ≥ 1) in the components of $\mathbf{y}(t)$. The approach to analyze the Jordan forms of A could answer this question, but since the algebraic multiplicities of the eigenvalues are unknown in general, it cannot be excluded that the components of $\mathbf{y}(t)$ could grow indefinitely in magnitude. In fact, we know that the Jordan blocks do introduce polynomials of order 1, at least, but they are removed from the solution in a surprising manner by the change of basis matrix Q (or P). In other words, all examples show that the change of basis matrix Q (or P) encodes the MCA condition in a way that higher-order generalized eigenvectors are mapped to zero.

To conclude, Paper IV explores the question about evolution in the Game of Teams, but it further formalizes the adaptive dynamics framework. It defines the dynamical process in a more rigorous way than the original articles. The main result is the correspondence between Nash equilibria in the team game and the stationary points of the adaptive dynamics.

Geometry and shape analysis

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Applications of shapes have been explored across many fields such as computer graphics and design, computer vision, and medical imaging. For instance, the anatomical manifestations of diseases are studied in the field of computational anatomy, initially pioneered by Grenander and Miller [27, 28]. Specifically, the alterations that diseases induce in the shapes of organs is tracked in order to provide early-stage diagnosis and scientific characterizations of the anatomical change. Shape analysis has proven to be a potent method for characterizing brain degeneration associated with neuro-cognitive impairments like Alzheimer’s or Huntington’s disease.

Shapes are usually expressed as curves, surfaces or images, and in such representations, the mathematical definition of a shape necessitates an infinite number of parameters. This requires the application of mathematical tools involving infinite-dimensional spaces, such as functional analysis, differential manifolds on general vector spaces and group theory. One such tool, which captures the infinite dimensionality as well as the group structure is the group of diffeomorphisms, that is, the set of “reversible” shape deformations.

Consider the shapes that are formed by deformations of a fixed *template* shape. Given another shape, called the *target* shape, one particular challenge is to identify the deformation that transforms the template into the

target. This target shape could for instance be an magnetic resonance imaging (MRI) image of tissue and the template which is supposed to match the target could be an older image of the same tissue region. For diseases such as Alzheimer's, following the shape changes of the tissue can help the diagnostic procedure [10]. The mathematical challenge is to create a suitable framework such that it is possible to construct a dynamics-driven process to find a shape transformation which sends the template close enough to the target while keeping the dynamics stable and producing a unique solution. To be geometrical, a transformation of a shape into another shape needs to follow a geometric dynamics. In this thesis, transformations of shapes are generated by an ODE problem, which is formulated on a differential manifold in such a way that the geometry is respected.

5.1 Template matching of images

This thesis focuses mainly on images as representations of shapes. A template image may describe gray-scale values for an image generated by MRI or computed tomography (CT). Given a real-valued image I , which is assumed to be a smooth function on some manifold M , let

$$I \circ \varphi^{-1}$$

be a deformation. Here, φ is an invertible map (a diffeomorphism) on M . The map φ^{-1} can be thought of as a change-of-coordinates, for instance with stretches and bends of some regions of the image. Let $\mathcal{D}(M)$ denote the group of all diffeomorphisms of M , namely smooth maps from M to itself with smooth inverses. The problem is to make sure that there is a way to find a single diffeomorphism φ among all diffeomorphisms in $\mathcal{D}(M)$ such that $I \circ \varphi^{-1}$ matches a given target. It is achieved in two steps:

1. A reasonable similarity measure is defined for every transformation $\varphi \in \mathcal{D}(M)$. A natural, but crude, choice is a function that is minimal if the target and the template are identical.
2. A differential equation is formulated on $\mathcal{D}(M)$. It is written using

notions from differential geometry, such that a template shape “flows” towards the target shape.

There are plenty of challenges: First, the action of $\mathcal{D}(M)$ on the space of functions in general is not transitive. That is, for any two given images, there is no guarantee that there exists a transformation such that they match perfectly. Moreover, in trying to find the best deformation of a template, the problem could be ill-posed if there are no restrictions on how crazy the diffeomorphisms are allowed to be.

Challenges such as these motivate the choice of similarity measure. Let $S : \mathcal{D}(M) \rightarrow \mathbb{R}$ be a function that is minimized when a template is completely deformed into the target. Then define another function $R : \mathcal{D}(M) \rightarrow \mathbb{R}$ that is minimal at the identity transformation. Let

$$E(\varphi) = S(\varphi) + \sigma R(\varphi), \quad \sigma > 0, \quad (5.1)$$

where σ is a parameter. This is the function which is to be minimized. The function S is a similarity term and R is a regularizer, and if σ is increased then the diffeomorphism φ is expected to be more regular in the sense that it is closer to the identity map in $\mathcal{D}(M)$. Assume the M is equipped with a Riemannian metric, g . Probably the most common function with the structure of (5.1) is

$$E(\varphi) = \|I_0 \circ \varphi^{-1} - I_1\|_{L^2}^2 + \sigma \text{dist}(\varphi, \text{id})^2 \quad (5.2)$$

where I_0 is the template image, I_1 is the target image, $\|\cdot\|_{L^2}$ is the L^2 norm on functions and $\text{dist}(\varphi, \text{id})$ is the geodesic distance on $\mathcal{D}(M)$ from the identity map to φ . Unfortunately, it is costly to use the geodesic distance as a regularizer on the group of diffeomorphisms. The main reason for this is that there is no closed form expression for the geodesic distance, so every time the diffeomorphism φ is changed, $\text{dist}(\varphi, \text{id})$ has to be computed algorithmically. Mathematically, however, (5.2) is beautifully connected to hydrodynamic-type partial differential equations via calculus of variations. Indeed, take the inner product on vector fields to be Sobolev H^k

$$\langle\langle v_t, v_t \rangle\rangle = \int_M g(Av_t, v_t) \mu_g, \quad \alpha > 0, \quad k \in \mathbb{N}, \quad A = (1 - \alpha \Delta)^k. \quad (5.3)$$

The geodesic distance $\text{dist}(\varphi, \text{id})$ is the infimum of $\int_0^1 \|v_t\|^2 dt$ over all paths that connect φ and the identity map and for which v_t is the vector field along the path. Via calculus of variations, an optimal v must fulfill the Euler-Poincaré equation on the diffeomorphism group (or *EPDiff* equation)

$$\dot{m} + Dm \cdot v + Dv^\top m + \text{div}(v)m = 0, \quad m = Av, \quad (5.4)$$

where $A = (1 - \alpha\Delta)^k$. The EPDiff equation with only one spatial dimension and $A = 1 - \Delta$ is the Camassa–Holm model for shallow water motion [11]. Geometrically these equations arise from the geodesic equation on $\mathcal{D}(M)$ with respect to the right-invariant Riemannian metric on $\mathcal{D}(M)$ induced by the inner product (5.3). Regularizing the problem using the geodesic distance $\text{dist}(\varphi, \text{id})$ is called large deformation diffeomorphic metric matching or *LDDMM*. Although computationally expensive, it provides a fully geometric solution to the matching problem. In an abstract group setting, the EPDiff equation can be written in terms of the co-adjoint action of a Lie group G , namely $\dot{v}^b = \text{ad}_v^* v^b$. It solves an abstract minimization problem which is formulated as (5.2) on general Lie groups, see Bruveris and Holm [10].

In order to avoid the lack of closed expressions in the matching problem, Paper III develops a numerical method via gradient descent. Assuming that the variational derivative of the energy function E on $\mathcal{D}(M)$ is given by explicit formulae one can consider the Riemannian gradient flow, defined by

$$\begin{aligned} \dot{\varphi} &= -\nabla E(\varphi) \\ \text{with } \varphi(0) &= \varphi_0 \end{aligned} \quad (5.5)$$

for some initial data $\varphi_0 \in \mathcal{D}(M)$. The simplest case, where E does not contain a regularization term, i.e., $\sigma = 0$ in (5.1), is called *greedy matching*. Typically greedy matching algorithms search for increasingly complicated diffeomorphisms in trying to achieve $I_0 \circ \varphi^{-1} = I_1$ regardless whether that is possible or not. On the other hand, the gradient flow can be very well-behaved if E is equipped with a reasonable regularizer. Gradient descent methods are not new to the matching problem [14, 5] but the

current setting identifies new structure in the gradient flow and derives new analytical results.

It turns out the a reasonable regularizer is the distance between the original metric g and its push-forward φ_*g using the L^2 -distance in the space of symmetric 2-forms,

$$R(\varphi) = \frac{1}{2} \|\varphi_*g - g\|_{L^2}^2. \quad (5.6)$$

By computing the variational derivative of $R(\varphi)$ we can avoid the costly algorithms associated with regularization via the Riemannian distance as in LDDMM. Still, we are able to retain the geometric properties, in particular that diffeomorphisms are generated by vector fields.

The regularization (5.6) is in a sense an outer distance on the space of diffeomorphisms, induced by the action of diffeomorphisms on the metrics. The distances are derived from an L^2 -metric on the space of Riemannian metrics and an H^1 metric on $\mathcal{D}(M)$, respectively [40, 12].

5.1.1 Greedy matching illustrates the idea

Consider the case that our configuration space is the space of smooth functions on M . The left action of $\mathcal{D}(M)$ on the smooth functions is the push-forward action

$$(\varphi, I) \mapsto I \circ \varphi^{-1}.$$

By differentiating the action map at the identity diffeomorphism, the infinitesimal action is obtained as $\xi \cdot I = -\iota_\xi dI$. The associated momentum map is then [10]

$$J(I, P) = -P \nabla I, \quad (5.7)$$

where ∇I is the gradient of I . As a similarity measure between images (or any functions), the L^2 type function $f(I) = \frac{1}{2} \|I - I_1\|^2$ is chosen, where I_1 is the fixed target function. Then $df = I - I_1$. To define an energy function on $\mathcal{D}(M)$, we choose $E(\varphi) = f(I_0 \circ \varphi^{-1})$ for a fixed template I_0 , that is,

$$E(\varphi) = \frac{1}{2} \|I_0 \circ \varphi^{-1} - I_1\|^2.$$

Then we differentiate E to find the differential dE and the corresponding gradient via the metric

$$\langle\langle \dot{\varphi}, \dot{\varphi} \rangle\rangle_{\varphi} = \langle\langle \xi \circ \varphi, \xi \circ \varphi \rangle\rangle_{\varphi} = \langle\langle \xi, \xi \rangle\rangle_e, \quad (5.8)$$

where $\langle\langle \cdot, \cdot \rangle\rangle_e$ is the inner product (5.3). Working on the L^2 -function space that defines the norm in the definition of E , one isolates $\xi = \dot{\varphi} \circ \varphi^{-1}$ and identifies the gradient ∇E as the vector that pairs with ξ . By this procedure, it turns out that

$$\nabla E(\varphi) = \left(- (1 - \alpha\Delta)^{-k} (I_0 \circ \varphi^{-1} - I_1) \nabla (I_0 \circ \varphi^{-1}) \right) \circ \varphi. \quad (5.9)$$

The gradient is defined by a vector ξ on the tangent space $T_e \mathcal{D}(M)$, which is transported by φ , that is, $\nabla E(\varphi) = \xi \circ \varphi$ for $A\xi = -(I_0 \circ \varphi^{-1} - I_1) \nabla (I_0 \circ \varphi^{-1})$, where $A = (1 - \alpha\Delta)^k$.

In Paper III, the structure of this gradient is identified for a general Lie group.

5.1.2 Sobolev setting in shape analysis

There is a tradeoff between the smoothness of operations and the analytical tools that are allowed on the group of diffeomorphisms (and in general for infinite-dimensional groups [62]). The smooth diffeomorphisms is a Fréchet Lie group, and it does not come with a fixed-point theorem and the consequential existence or uniqueness theorems for ordinary differential equations. In particular, the gradient flow equation $\dot{\varphi} = -\nabla E(\varphi)$, where ∇E is given by (5.9) is not guaranteed to have a well-defined solution even though that would be immediate in a finite-dimensional Lie group setting. In order to retain a Hilbert manifold setting, the group of smooth diffeomorphisms is extended via Sobolev completions. The resulting completion, $\mathcal{D}^s(M)$, is a Hilbert manifold if $s > \dim(M)/2 + 1$, but the Lie group structure is lost. For instance, the composition map is only continuous. This tradeoff situation implies that the existence of a gradient flow (which is one of the main results of Paper III) is not a trivial application of the general Lie group theory.

The idea that saves the situation is that even though the group structure is not smooth, the gradient may still be a smooth vector field. The smoothness of the gradient is a consequence of its geometric structure. It can be decomposed into vector fields, which are smooth “transportations” on the group of diffeomorphisms. Such transportations are very suitable for building compositions, a fact that was well explored by Ebin and Marsden [21] and which Paper III applies to the current gradient flow problem.

The tangent bundle of $\mathcal{D}^s(M)$ is the union of tangent spaces on the form

$$T_\varphi \mathcal{D}^s(M) = \{u \in H^s(M, TM) : \pi \circ u = \varphi\},$$

where π is the natural projection. That is, every vector on $T\mathcal{D}^s(M)$ can be represented as $v \circ \varphi$ for some $v \in \mathfrak{X}^s(M)$. To the right translation $\varphi \mapsto v \circ \varphi$ applies the “omega lemma” [21], which seems to imply that the vector fields need sufficient smoothness to be transported by right translation. Moreover, gradients such as (5.9) involve the inversion map $\varphi \mapsto \varphi^{-1}$, which is only continuous on the Sobolev class diffeomorphisms $\mathcal{D}^s(M)$. However, it is the composition structure of the gradient flow that provides the smoothness that is needed for existence theorems. It is illustrated by the following lemma, which is from Paper III.

Lemma 5.1. *Let $T\mathcal{D}^{s-k}(M) \upharpoonright \mathcal{D}^s(M)$ denote the restriction of the tangent bundle $T\mathcal{D}^{s-k}(M)$ to the base $\mathcal{D}^s(M)$. Given a (non-linear) 2^{nd} order differential operator $F : \mathcal{D}^s(M) \rightarrow \mathfrak{X}^{s-2}(M)$, define*

$$\tilde{F} : \mathcal{D}^s(M) \rightarrow T\mathcal{D}^{s-2}(M) \upharpoonright \mathcal{D}^s(M) \quad (5.10)$$

$$\varphi \mapsto (\varphi, F(\varphi^{-1}) \circ \varphi). \quad (5.11)$$

If $s > 2 + \frac{1}{2} \dim M$ then $\tilde{F}$ is smooth.

Remark. The inversion map on $\mathcal{D}^s(M)$ is not smooth, so it is indeed the composition structure of $\tilde{F}$ that saves the day. If F is of k^{th} order, the condition on s would be $s > k + \frac{1}{2} \dim M$ with similar results.

Proof. In local coordinates given by smooth functions f_i on some open subset of $\mathbb{R}^n \times \mathbb{R}^{n \times n} \times \mathbb{R}^{n \times n \times n}$,

$$F(\varphi^{-1})(x)_i = f_i(\varphi^{-1}(x), D\varphi^{-1}(x), D^2\varphi^{-1}(x))$$

where $n = \dim M$, and $D\varphi^{-1}$ is (in coordinates) the matrix of derivatives: $D\varphi^{-1}(x)_j^i = \frac{\partial \varphi_i^{-1}}{\partial x^j}(x)$. Now, consider the composition $F(\varphi^{-1}) \circ \varphi$. The mapping

$$\mathcal{D}^s(M) \rightarrow H^{s-1}(M), \quad \varphi \mapsto \frac{\partial \varphi_i^{-1}}{\partial x^j} \circ \varphi$$

is smooth because $D\varphi^{-1} \circ \varphi = (D\varphi)^{-1}$ and matrix inversion is a smooth, point-wise operation. Similarly, the second-order derivatives can be written as matrix inversions and multiplications: $D^2\varphi^{-1} \circ \varphi = D(D\varphi)^{-1}(D\varphi)^{-1}$. Now $\varphi \mapsto \partial^2 \varphi_i / \partial x^j \partial x^k \circ \varphi$ as a mapping $\mathcal{D}^s(M) \rightarrow H^{s-2}(M)$ is smooth if $s > 2 + n/2$ since in that case $D(D\varphi)^{-1}$ is above the Sobolev embedding threshold, which implies that it can be smoothly multiplied with elements in $H^{s-1}(M)$. Since the coordinate maps f_i are smooth mappings, the omega lemma implies that $\tilde{F}$ is a smooth bundle map. $\square$

This lemma has an equivalent for operators on densities in Lemma 27 of Modin and Bauer [4]. Ebin and Marsden [21] worked out the same smoothness results for, among other operators, the differential d and the co-differential δ .

The deformations imposed by diffeomorphisms are quantified in the space of symmetric $(0, 2)$ -tensor fields. Let $S_{(0,2)}^{s-1}(M)$ be the space of symmetric 2-forms of class H^{s-1} with $s > 1 + \frac{1}{2} \dim M$. Then, if $C^0\text{Met}(M)$ is the space of continuous Riemannian metric on M , define

$$\text{Met}^{s-1}(M) = C^0\text{Met}(M) \cap S_{(0,2)}^{s-1}(M).$$

Metrics on M of class H^{s-1} constitute an open set of the bundle of symmetric tensor fields of type $(0, 2)$ on M . In particular, it is a smooth Hilbert manifold [73]. The tangent space is $T\text{Met}^{s-1}(M) \simeq \text{Met}^{s-1}(M) \times S_{(0,2)}^{s-1}$. Instead of using the canonical metric on $\text{Met}^{s-1}(M)$, the so-called Ebin metric [19], the framework in Paper III is using an L^2 type distance to make the computations less costly in applications such as image matching. This L^2 distance is based on the L^2 inner product on $S_{(0,2)}^{s-1}$,

$$\langle h, k \rangle = \int_M g(h, k) \mu_g = \int_M h^{ij} k_{ij} \mu_g$$

and the distance $\text{dist}(h, k) = \|h - k\|^2$ for any two metrics $h, k \in \text{Met}^{s-1}(M)$. As already mentioned, the distance which is used to regularize the gradient flow is the distance from the “background metric” to the pushforward metric, that is $\text{dist}(\varphi_*g, g)$.

In the above setup, we have defined diffeomorphisms of class H^s and metrics of class H^{s-1} , though s is a smoothness parameter of choice. It makes sense, however, to reserve s for the diffeomorphisms and keep track of the -1 in the notation, because in the current application, the action of the diffeomorphisms on the metrics determine the smoothness of the metrics. The original metric g is smooth, but the pushforward metric (that is, the modelled deformations) are H^{s-1} smooth. The smoothness reduction by one integer unit is due to the differentials in the definition of the pushforward metric.

5.2 Main results of Paper III

One main result of Paper III concerns the existence and uniqueness of a gradient flow for the matching problem of images. Another central result is the geometric structure of certain gradient flows on Lie groups. That is, the matching problem is approached as in the above sections but also with generalizations of the equations such as (5.9). To that end, let Q be a shape representation, which can be selected according to the application, as shapes can be represented in multiple ways. To model a deformation of a shape, q , let the (left) action of a group element $g \in G$ on the shape, $g \cdot q$, represent a deformation of the original shape. The goal is to identify which transformation g that generates a shape such that it is similar to a given target.

A central technique is the analysis on Sobolev spaces, with methods inspired by the works of Ebin and Marsden [21] on hydrodynamics equations, which in Paper III is applied to a gradient system. The first step towards analysing the gradient flow is to identify the geometric components of it. The second step is to analyze the Sobolev space regularity of the gradient flow. In identifying the geometric structure of the gradient flow, it is found

that the gradient of $E : G \rightarrow \mathbb{R}$ is a composition of mappings:

$$\nabla E(g) = \xi \cdot g, \quad \text{where } A\xi = J(g \cdot q_0, df(g \cdot q_0)) \quad (5.12)$$

where $f : Q \rightarrow \mathbb{R}$ is a function on the configuration manifold Q , A is the inertia operator on the Lie algebra and J is the momentum map of the cotangent lifted left action of $\mathcal{D}(M)$ on Q . To carry on the procedure, Equation (5.12) is decomposed into smooth vector fields from which the existence and uniqueness of the gradient flow can be derived. See Section 5 of Paper III for details on the proofs. Section 5.2.1 outlines the structure of Equation (5.12) and Section 5.2.2 describes the existence and uniqueness results.

5.2.1 The gradient flow geometry on a Lie group

From the recent works of K. Modin and collaborators, including Paper III, the geometric structure of Riemannian gradient flows confined to group orbits has been uncovered [43]. In this section, we leave out the analytical questions in order to focus on the geometric structure of the gradient flow. To that end, let G be a Lie group (or a Fréchet–Lie group in the infinite-dimensional case) acting from the left on a “shape space”, which is another manifold Q , possibly infinite-dimensional. Assume that the action map is smooth.

The *infinitesimal action* corresponding to a Lie algebra $\mathfrak{g}$ is given by differentiating the action map $g \cdot q$ with respect to g at the identity in the direction of some vector field v . The resulting infinitesimal action of $v \in \mathfrak{g}$ on $q \in Q$ is denoted $v \cdot q$. Keeping $v \in \mathfrak{g}$ fixed defines a vector field $Q \rightarrow TQ$, given by $q \mapsto v \cdot q$. On the other hand, the mapping $v \mapsto v \cdot q$ is linear and it motivates the following:

Definition 5.1. The *momentum map* $J : T^*Q \rightarrow \mathfrak{g}^*$ is defined by

$$\langle J(q, p), v \rangle = \langle p, v \cdot q \rangle \quad \forall v \in \mathfrak{g}, \quad (5.13)$$

where T^*Q denotes the cotangent bundle of Q .

Here, if Q is an infinite-dimensional Fréchet manifold, the cotangent bundle T^*Q is given in terms of the *regular dual* [44], defined so that $T_q^*Q \simeq T_qQ$.

If the tangent space T_eG at the identity of G (i.e. the Lie algebra) has an inner product $\langle\langle \cdot, \cdot \rangle\rangle_e$, then it determines a right invariant metric on TG by means of the right action. We remark that Q is not assumed to be Riemannian, but the orbit $G \cdot q = \{g \cdot q \mid g \in G\}$ will inherit a Riemannian metric from G , as shown by Khesin and Modin [43].

Let $q_0 \in Q$ and let $f: Q \rightarrow \mathbb{R}$ be a function which is to be minimized on Q . Specifically, we are interested in finding the minimum of f on the G -orbit starting at q_0 and thereby minimize the function $E: G \rightarrow \mathbb{R}$ defined by

$$E(g) = f(g \cdot q_0). \quad (5.14)$$

If G is equipped with a right-invariant Riemannian metric $\langle\langle \cdot, \cdot \rangle\rangle$ defined by

$$\langle\langle u \cdot g, v \cdot g \rangle\rangle_g = \langle Au, v \rangle$$

where A is the inertia operator $A: \mathfrak{g} \rightarrow \mathfrak{g}^*$, the corresponding gradient vector field ∇E on G is given by

$$\langle\langle \nabla E(g), \dot{g} \rangle\rangle_g = \langle dE, \dot{g} \rangle. \quad (5.15)$$

The aim is to solve the minimization problem by considering the gradient flow

$$\dot{g} = -\nabla E(g). \quad (5.16)$$

Theorem 5.2. *The gradient ∇E is given by*

$$\nabla E(g) = \xi \cdot g. \quad (5.17)$$

where $\xi \in \mathfrak{g}$ is given by

$$\xi = A^{-1}J(g \cdot q_0, df(g \cdot q_0)). \quad (5.18)$$

Proof. Let $\dot{g} = \xi \cdot g$. By definition of the gradient and the chain rule

$$\langle\langle \nabla E, \dot{g} \rangle\rangle_g = \langle dE, \xi \cdot g \rangle = \frac{d}{dt}E(g) = \langle df, \xi \cdot (g \cdot q_0) \rangle.$$

From the definition of the momentum map it follows that

$$\langle\langle \nabla E, \dot{g} \rangle\rangle_g = \langle J(g \cdot q_0, df), \xi \rangle = \langle\langle A^{-1}J(g \cdot q_0, df), \xi \rangle\rangle_e$$

The result follows since the metric is right invariant. $\square$

This theorem provides the geometry of the gradient flow. As shown by Khesin and Modin [43], the resulting gradient flow (5.16) induces a gradient flow on the G -orbit of q_0 , given by

$$\dot{q} = -u(q) \cdot q \quad (5.19)$$

where $u(q) = A^{-1}J(q, df(q))$. Khesin and Modin derives a double-bracket flow of vorticity functions for the incompressible Euler equations on the 2-dimensional sphere using this result.

The gradient flow that follows this treatment will have some of the properties that are well-known in similar settings, such as the following. Consider the Riemannian distance on G , given by integration along the geodesic between two group elements $g_0, g_1 \in G$,

$$d(g_0, g_1) = \inf_{\gamma} \int_0^1 \|v(t)\|_A dt, \quad \dot{\gamma} = v \circ \gamma, \quad (5.20)$$

where the infimum is taken over all smooth curves $\gamma : [0, 1] \rightarrow G$ constrained by $\gamma(0) = g_0$ and $\gamma(1) = g_1$. Here, $\|v\|_A$ is the norm induced by the inner product (5.3). Then, using the right-invariance of the metric,

$$\frac{d}{dt}E(\gamma) = \langle\langle \nabla E(\gamma), \dot{\gamma} \rangle\rangle_{\gamma} = -\langle Av, v \rangle = -\|v\|_A^2. \quad (5.21)$$

It follows that the gradient flow decreases the energy E along its path. From a computational point of view, it is reasonable to have a stopping criteria based on the decrease. In Section 5.2.3, this will be discussed.

5.2.2 Well-posedness of the gradient flow

The above derivation of the gradient flow equation's structure in terms of the momentum map does not specify when the gradient flow exists, but this section will. Theorem 2.7 in Paper III proves the well-posedness of this gradient flow. Here, we repeat it:

Theorem 5.3. *Let $E : G \rightarrow [0, \infty)$ be such that the gradient vector field ∇E on G satisfies a local Lipschitz condition. Then the gradient flow $\dot{\gamma} = -\nabla E(\gamma)$ with initial data $\gamma(0) \in G$ admits a unique global solution.*

Key to the proof of this theorem is to show that the flow is Hölder continuous. For details, see Paper III.

In the case when Q is the manifold of images and metrics, $Q = H^s(M, \mathbb{R}) \times \text{Met}^{s-1}(M)$, the push-forward action is, respectively,

$$(\varphi, f) \mapsto f \circ \varphi^{-1} \quad \text{and} \quad (\varphi, g) \mapsto \varphi_* g,$$

where the push-forward metric is as in Section 2.5. The momentum map associated to the action on functions in $H^s(M, \mathbb{R})$ is (5.7) while the momentum map associated to the action on the metrics in $\text{Met}^{s-1}(M)$ is

$$J(h, \pi) = 2\text{tr}_h(\text{div } \pi) + \text{tr}_{u,v}(2\pi(u, v)\nabla h(u, \cdot, v) - \pi(u, v)\nabla h(\cdot, u, v)). \quad (5.22)$$

This can be seen as a bi-linear divergence-type differential operator. In Paper III, $\text{div}_h(\pi) = \text{tr}_h(\text{div } \pi) + \frac{1}{2}\text{tr}_{u,v}(2\pi(u, v)\nabla h(u, \cdot, v) - \pi(u, v)\nabla h(\cdot, u, v))$ is called the divergence of $(0, 2)$ -tensors.

Next, consider

$$E(\varphi) = \frac{1}{2}\|I_0 \circ \varphi^{-1} - I_1\|^2 + \frac{\sigma}{2}\|\varphi_* g - g\|^2$$

where the norms are defined on $H^s(M, \mathbb{R})$ and $\text{Met}^{s-1}(M)$, respectively. This is the energy functional that balances between the similarity of $I_0 \circ \varphi^{-1}$ and I_1 on the one hand and the regularity of $\varphi_* g$ on the other hand. If the parameter σ is increased then E gets more sensitive to deviations of φ from the identity mapping.

Theorem 5.4. *Let $\mathfrak{X}^{s-2}(M)$ be the vector fields on M of Sobolev type H^{s-2} and let $S_{0,2}^{s-1}(M)$ be the space of summetric $(0, 2)$ -tensor fields on M of Sobolev type H^{s-1} . The gradient of E with respect to the right-invariant Riemannian metric on $\mathcal{D}^s(M)$ defined by (5.3) and (5.8) is*

$$\nabla E(\varphi) = v \circ \varphi, \quad Av = J(\varphi_* I_0, \varphi_* g, \delta_I f, \delta_h f)$$

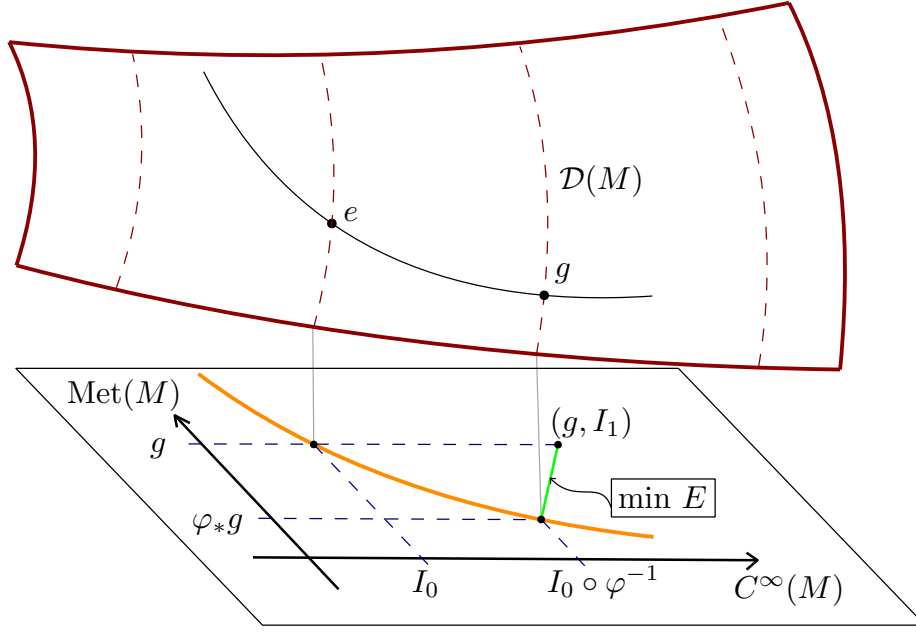


Figure 5.1: The gradient flow translates the identity $e \in \mathcal{D}(M)$ into $\varphi \in \mathcal{D}(M)$, and the diffeomorphism φ acts on both metrics and functions.

where $J : T^*Q \rightarrow \mathfrak{X}^*(M)$ is identified as the mapping

$$H^s(M, \mathbb{R}) \times \text{Met}^{s-1}(M) \times H^s(M, \mathbb{R}) \times S_{0,2}^{s-1}(M) \rightarrow \mathfrak{X}^{s-2}(M)$$

$$(I, h, P, \pi) \mapsto -P\nabla I + 2 \operatorname{div}_h(\pi).$$

Here, $-P\nabla I$ is the momentum map of the action of $\mathcal{D}^s(M)$ on functions, Equation (5.7), while $2 \operatorname{div}_h(\pi)$ is defined by $J(h, \pi) = 2 \operatorname{div}_h(\pi)$ in Equation (5.22).

The momentum map of Theorem 5.4 is a sum of two separate momentum maps. That is, the structure of the direct product between functions and metrics is carried over to the cotangent space by summation. The flow evolves on the group of diffeomorphisms and traces a path on the configuration space, see Figure 5.1. The target is $(g, I_1) \in Q$ but the action orbit can usually only achieve to come close to it.

Corollary 5.4.1. Applying 5.4 to $E(\varphi) = f(I_0 \circ \varphi^{-1}, \varphi_* g)$, where

$$f(I, h) = \frac{1}{2} \|I - I_1\|^2 + \frac{\sigma}{2} \|h - g\|^2,$$

the gradient flow is defined by $\dot{\varphi} = -\nabla E(\varphi)$ where

$$\begin{aligned}\nabla E(\varphi) &= v \circ \varphi \\ (1 - \alpha\Delta)^k v &= -(I_0 \circ \varphi^{-1} - I_1)\nabla(I_0 \circ \varphi^{-1}) + 2\sigma \operatorname{div}_{\varphi_*g}(\varphi_*g - g)\end{aligned}$$

Theorem 5.4 provides a closed expression for the momentum map of the pushforward action on the configuration manifold $H^s(M, \mathbb{R}) \times \operatorname{Met}^{s-1}(M)$. One important implication is that the gradient flow $\nabla E(\varphi) = v \circ \varphi$ can be computed at any time along the integration curve, starting from, say, $\varphi(0) = \operatorname{id}$. Compared to the LDDMM setting, as explained above, it is computationally faster to solve the gradient flow using these formulas. The setting in Proposition 5.4 allows these closed expressions much due to the choice of regularization, that is, the L^2 -type distance $\|h_1 - h_2\|$ on the space of metrics.

The next result is the existence of the gradient flow. For this, assume that the fixed functions I_0 and I_1 are C^∞ -smooth. Let $s > 2 + \frac{1}{2} \dim M$.

Theorem 5.5. *For each initial datum $\varphi_0 \in \mathcal{D}^s(M)$, there exists a maximal $T > 0$ and unique curves $\varphi : [0, T) \rightarrow \mathcal{D}^s(M)$ and $v : [0, T) \rightarrow T_{\operatorname{id}}\mathcal{D}^s(M)$ with $\varphi(0) = \varphi_0$ that fulfills the gradient flow equation in Corollary 5.4.1. The solution depends smoothly on the initial data (in the Hilbert manifold topology of $\mathcal{D}^s(M)$). Furthermore, if $k \geq s$ then the maximal time T is infinite, that is, the flow is globally well posed.*

Remark. The well-posedness does not depend on σ . However, the value of σ significantly impacts how the images appear along the gradient flow.

Remark. It is very useful that the order of the inertia operator $A = (1 - \alpha\Delta)^k$, determines whether the flow is globally well-posed or only locally. The inertia operator is freely chosen to suit this requirement; it is part of the computational framework. Note that A can be any invertible elliptic differential operator of order ≥ 2 .

The key to the proof of Theorem 5.5 is to show that $\dot{\varphi} = -\nabla E(\varphi)$ from Corollary 5.4.1 is an ordinary differential equation defined by a smooth vector field on the infinite-dimensional Hilbert manifold $\mathcal{D}^s(M)$. Once this

is established, local existence follows from the Picard–Lindelöf theorem on Banach manifolds [47]. Global well-posedness follows precisely by the same steps as in the finite-dimensional case. If $k \geq s$ then the Riemannian metric defined by the inertia operator A is strong enough to dominate the topology of $\mathcal{D}(M)$. The estimates obtained as in the finite-dimensional case exclude the possibility of blowup as $t \rightarrow T$. Since the general theory of maximal solutions of ODEs is valid also in the Banach category, we conclude that $T = \infty$ in this case.

5.2.3 Example on the 2-dimensional flat torus

For $M = \mathbb{T}^2$, the 2-dimensional flat torus, the image matching methods in this chapter can be implemented to produce figures such as Figure 5.2. Here, the toy example matching problem is the deformation of the letter I with target letter C. The pixel values of the image are moved around via the map φ^{-1} , then displayed. The warp figure in Figure 5.2 is the original coordinate system (horizontal and vertical lines) mapped via φ^{-1} . Since φ is a diffeomorphism, it does not destroy structures that would make the warp impossible to reverse. For instance, two of the corners of the letter I are still visible on the sides of the letter C in the warped image: one on the upper-left side and one on the lower-left side. The flow, which starts at $\varphi = \text{id}$, is allowed to evolve until the energy $E(\varphi)$ stabilizes at a significantly lower value compared to $E(\text{id})$. As can be seen in Figure 5.3, which corresponds to the deformation in Figure 5.2, the energy decreases rapidly during the first 100 iterations. This rapid decrease of E is usually caused by linear translations in the case of the flat torus. After the first 100 iterations there is a region of slower decay of energy, which often corresponds to non-rigid deformations which are “impossible” on the space of diffeomorphisms, such as the removal of corners, or in other examples the disappearance of entire regions. If this matching algorithm should be applied to, say, medical image analysis, it can be expected that the stopping criteria need to be automatic. They could be taken on the rate of decrease of the energy $E(\varphi)$. The convergence of E is fast compared to the LDDMM method. Beg *et al.* [5] compared the LDDMM method to the greedy matching algorithm and found that the LDDMM method

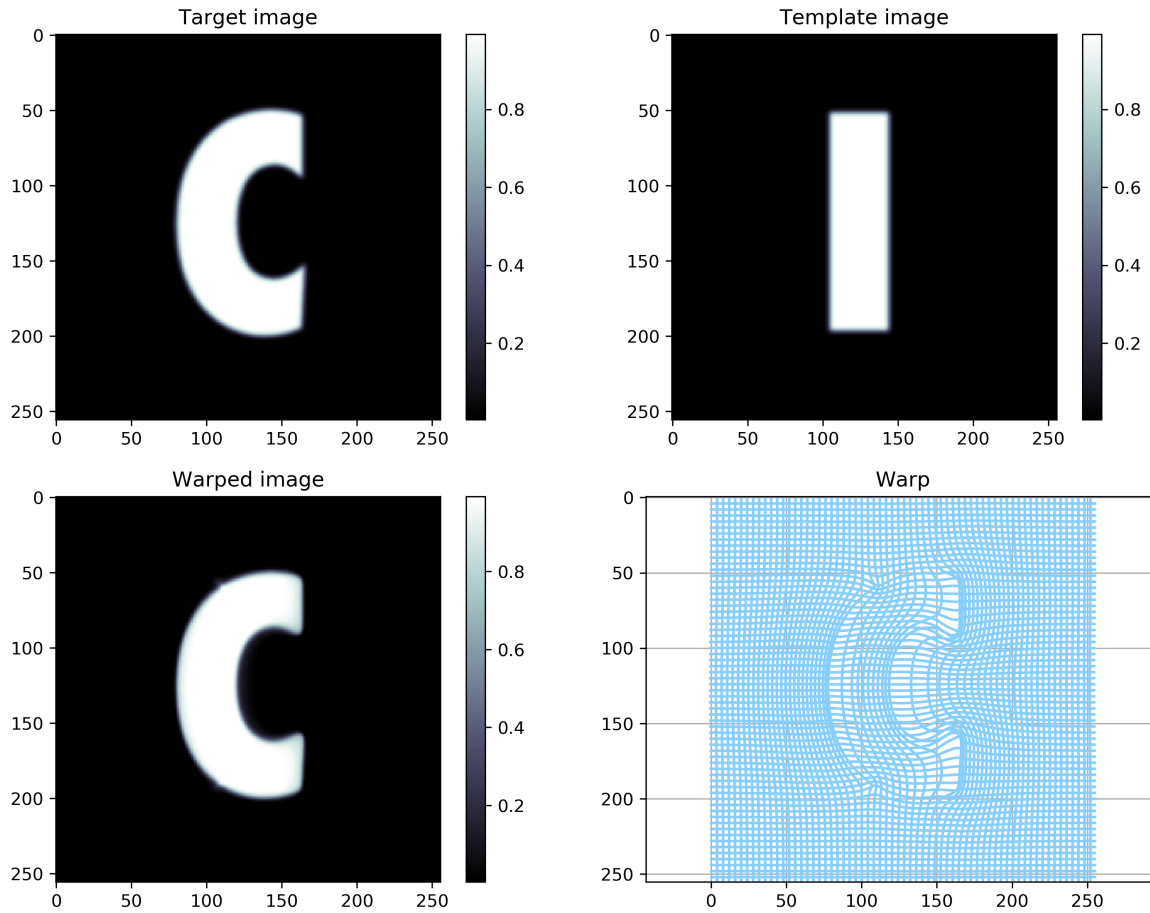


Figure 5.2: The warp of a template function, trying to replicate the target.

is about ten times slower for rigid deformations and around 100 times slower for non-rigid image matching. The gradient flow method of Paper III experiences a slow-down due to the regularization on the order of the greedy matching. That is, the non-rigid image matching in Paper III is orders of magnitudes faster than the LDDMM.

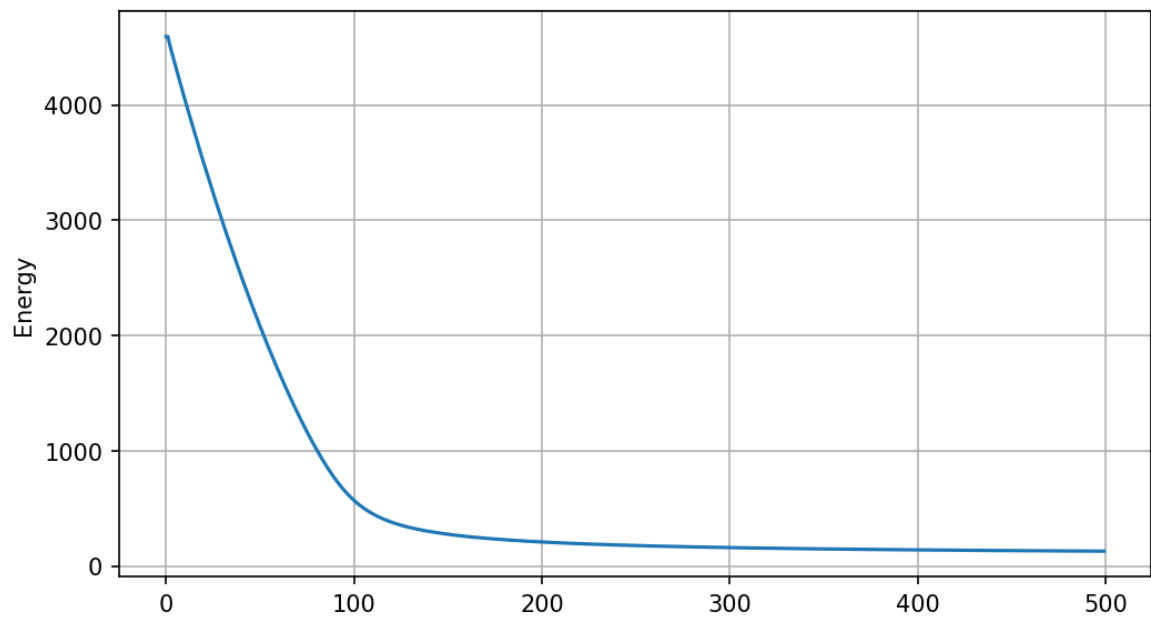


Figure 5.3: The energy $E(\varphi)$ as the gradient flow φ evolves.

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