Inferring eco-evolutionary feedbacks from time series data using neural ordinary differential equations

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Abstract

Ecological and evolutionary dynamics were thought to operate on different time scales. Recent evidence showed that evolution could be rapid enough to interplay with ecological dynamics and form eco-evolutionary feedbacks. These feedbacks are hard to identify in nature, due to the complexity of the mechanisms and the difficulty of obtaining phenotypic, demographic, and environmental variables. We lack quantitative evidence on feedback effects in real systems, which prevents us from painting a complete view of feedback architectures. We develop a mathematical framework, neural ordinary differential equations (NODEs), to quantify feedbacks from time series data of the evolutionary, ecological, and environmental variables in the system. The framework combines ordinary differential equations and artificial neural networks, to identify, non-parametrically, drivers of evolutionary and ecological dynamics, and relies on the Geber method to recover the contribution of ecological change to evolution, and vice versa. We apply the technique to recover the coupling between the dynamics of three species in a prey-predator system. We find that main interactions, between the prey and top predator are conserved across replicates, while weaker interactions, between the intermediate predator and the other species, are not. We also apply the technique to recover eco-evolutionary feedbacks in two of Darwin's finches species. We find that feedbacks involve a direct coupling between population dynamics and phenotypic change in only one of the species, while the other involves a coupling with resource levels. Our work demonstrates the potential of NODEs in uncovering drivers of dynamics in systems where prior mechanistic knowledge is lacking, and shows the importance of indirect effects in driving eco-evolutionary feedbacks in nature.

Authors contributions

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Designed all studies and methods. Performed all analyses. Wrote all manuscripts.

Ben C. Sheldon

Directed the research. Provided detailed comments on all manuscripts.

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Directed the research. Provided detailed comments on all manuscripts.

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Part I

Chapter 1: Introduction and literature review

Introduction and literature review

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1 Introduction and literature review

1.1 Eco-evolutionary dynamics

The field of eco-evolutionary dynamics aims at understanding the drivers of ecological and evolutionary change (Pelletier, Garant, and Hendry 2009). Ecological and evolutionary change operate on ecological and evolutionary variables. In the context of eco-evolutionary dynamics, ecological variables usually describe the state of populations, or communities, such as the number or density of individuals, or the amount of biomass (Fussmann, Loreau, and Abrams 2007). Change in these variables is caused by demographic events, such as the death and birth of individuals (e.g. Dieckmann, Marrown, and Law 1995). Evolutionary variables usually correspond to genotype frequencies in the population (Fussmann, Loreau, and Abrams 2007). Genotypes correspond to the genetic structures which, along with the environment, govern the expression of phenotypes. Phenotypes are properties of individuals that influence the way they interact with other organisms (prey, competitors, predators), and how they are affected by their abiotic environment (e.g. temperature, rainfall). Phenotypic change arises through evolution, heritable changes in the genetic architecture of the traits (Fussmann, Loreau, and Abrams 2007), and/or plasticity, which involves non-heritable changes in traits within the lifetime of an individual (Hendry 2013; Kokko et al. 2017). In this sense, the phenotype is the nexus of eco-evolutionary dynamics (Hendry 2013), because effects of the genetic architecture on ecology, and effects of ecology on the genetic architecture, are both mediated by the phenotype.

Historically, ecological and evolutionary dynamics were studied independently. This is due to the

fact that evolution was thought to operate on geological time scales, while ecological change would take place within the lifetime of an individual (TerHorst et al. 2018). The ecological and evolutionary state of a system, namely the species composition, the state of populations, the properties of individuals, would drive evolutionary change. However, the evolutionary change thereby induced would be too slow to feed back on ecological change (Fussmann, Loreau, and Abrams 2007; Pelletier, Garant, and Hendry 2009). In other words, in the eyes of ecology, evolution would be so slow that the evolutionary state of the system could be considered constant (Reznick 2016), and in the eyes of evolution, ecological change would be so fast that the new ecological equilibrium would be reached instantly (Dieckmann, Marrown, and Law 1995). Fields such as adaptive dynamics would hence consider that the ecological state of a system would always reach an equilibrium enforced by the current evolutionary state (Dieckmann, Marrown, and Law 1995). Similarly, classical ecological models, such as the Lotka-Volterra model would consider vital rates, determined by the phenotypes of individuals, to be constant (Reznick 2016).

It was demonstrated empirically in the 90s that evolution could be fast enough to interplay with ecological change (Reznick, Bryga, and Endler 1990; Grant and Grant 1993). The evidence came from two iconic systems, the guppy (*Poecilia reticulata*) fish system in Trinidad (Reznick, Bryga, and Endler 1990), and the Darwin's finches (*Geospiza fortis*, *Geospiza scandens*) system in the Galapagos (Grant and Grant 1993). In the guppy system, David Reznick and colleagues transferred guppies from high predation sites to low predation sites. They showed that in the course of 10 years, the fish would switch from a high predation phenotype to a low predation one, as they would grow

to greater body lengths, and produce fewer offspring (Reznick 2016). In the Darwin's finches system, Peter and Rosemary Grant monitored a population of common cactus finch (*G. scandens*) and medium ground finch (*G. fortis*) located on Daphne Major island in the Galapagos. They reported that an exceptionally strong el Nino event in 1983 depleted the large seeds available to the finches, in favour of small seeds. Following this event, they observed that the beak of the finches became smaller and more pointed within 3 years (Grant and Grant 1993).

These pioneering studies were followed by a large body of work on fast evolution across a variety of taxa, in invertebrates (Yoshida et al. 2003; Waasdorp et al. 2015; Frickel, Sieber, and Becks 2016; Siepielski et al. 2016; Stewart et al. 2017; Sruti et al. 2017; Crespi et al. 2018), fish (Olsen et al. 2005), mammals (Pelletier et al. 2007; Ezard, Côté, and Pelletier 2009; Coulson et al. 2011; Pigeon et al. 2017), and birds (Garant et al. 2004; Beausoleil et al. 2019). Overall, the work brought key insights into fast evolution, first by confirming that fast heritable trait change was common in nature (e.g. Reznick, Bryga, and Endler 1990; Grant and Grant 1993; Pelletier, Garant, and Hendry 2009; Schoener 2011). In natural fish communities, intense size selective fisheries of the Canadian cod led to an evolutionary response towards smaller body size at maturity within a matter of years (Olsen et al. 2005). It also established that rapid evolution could impact the dynamics and state of populations (e.g. Yoshida et al. 2003; Hairston et al. 2005; Pelletier et al. 2007; Becks et al. 2012; Reznick 2016). For instance in a microcosm experiment, Yoshida and colleagues showed that rapid evolution of anti-predator clumping behaviour of algae could slow down the frequency of prey-predator oscillations (Yoshida et al. 2003). More recently, rapid evolution was shown to

alter the state of other ecosystem components (e.g. Bassar et al. 2010; Bassar et al. 2012; Bassar et al. 2015; Reznick 2016; Simon et al. 2017). The evolution of guppy fish is thought to involve complex effects on nutrient levels, decomposition rates, algal and invertebrate standing biomass (Bassar et al. 2012).

1.2 Eco-evolutionary feedbacks

The work established that evolution could be fast enough to interplay with ecological change, thereby forming so-called eco-evolutionary feedbacks (Post and Palkovacs 2009; Pelletier, Garant, and Hendry 2009; Schoener 2011). Eco-evolutionary feedbacks correspond to the pathways, namely effects between ecological and evolutionary variables, through which ecological and evolutionary dynamics are coupled. They arise when changes in the genetic, phenotypic, and ecological state of communities occur conjointly and interdependently (Figure 1). In such a case, evolutionary change accounts for changes in ecological variables, and in turn, ecological change accounts for changes in evolutionary variables. From a conceptual perspective, the structure of eco-evolutionary feedbacks can be characterised as a set of state variables, evolutionary, ecological, or environmental (i.e. abiotic) in nature, and interactions, namely pathways for effects between these variables. Throughout this thesis, dynamical processes correspond to functional representations describing the set of variables and interactions that drive the dynamics of a given variable, or of the entire system. Each process can be explained by several different mechanisms, which can be understood as particular mathematical representations of the processes.

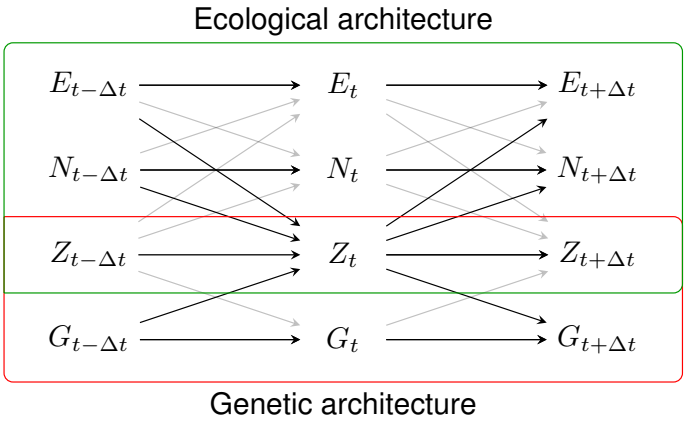

Figure 1: Conceptual view of the eco-evolutionary feedback loop. E is the environment state vector, N is the population state vector, Z is the trait state vector, and G the genetic state vector. Arrows correspond to functional relationships between states. Grey arrows are part of former and subsequent feedback loops. The red and green box highlight the genetic and ecological architecture of the system.

Feedbacks are highly complex to study as they require the integration of (i) the ecological architecture of ecosystems (Figure 1, green box), which consists of multiple interacting organisms (N) (TerHorst et al. 2018), characterized by multiple interdependent traits (Z) (Kokko et al. 2017), in a spatially and temporally variable environment (E) (Rodríguez-Verdugo, Buckley, and Stapley 2017), and (ii) the genetic architecture underlying each trait (Figure 1, red box), which may involve multiple genes (G), pleiotropic interactions, linkage, modularity, epigenetics, plasticity (Kokko et al. 2017), and alternative molecular pathways encoding the same phenotype (Becks et al. 2012).

A simple example of feedback can be found in the algae-rotifer prey-predator system (Yoshida et al. 2003). The evolution of clump predator defense by algae is influenced by predator density. Changes in the propensity of algae to form clumps affect the growth rate of both the algae and its rotifer predator, and thereby alters the density of prey and predator in the system. In turn, changes in population densities feed back on the dynamics of the defense trait by increasing or decreasing selection (Yoshida et al. 2003; Becks et al. 2012).

A similar eco-evolutionary feedback has been hinted at in the guppy fish (Reznick 2016; Reznick et al. 2019). The introduction of guppy fish from high-predation to low-predation sites initially resulted in a drastic increase of the guppy fish population density, in association with a depletion of the invertebrate biomass, their primary food source. Guppies then turned to consuming algae, for lack of invertebrates. Reznick and colleagues then showed that the evolution of the low-predation phenotype by guppies was delayed, as it followed the population density peak (Reznick et al. 2019).

They hence argued that the rapid evolution of guppies was more likely a response to the impact of guppies on their own environment, rather than an immediate response to experiencing the low-predation environment. In their view, the evolutionary response of guppies in that system hence stemmed from an eco-evolutionary feedback between population density and phenotypic change (Bassar et al. 2013).

1.3 Knowledge gaps

Overall, we have indirect evidence supporting the existence of feedbacks in natural systems (Wooliver et al. 2018), but we still lack direct quantitative evidence documenting the strength of the different pathways linking ecological and evolutionary change. This is due to the fact that most studies have focussed either on the eco-to-evo or the evo-to-eco pathway for effects, in a handful of well-studied systems (Hendry 2019). This is also a consequence of the lack of suitable, and consensual, methodology to quantify feedbacks (Benthem et al. 2017; Hendry 2019). Systems in which we have identified full feedbacks are rare, especially in nature (Brunner et al. 2019). Even in the most studied systems, such as the guppy and the Darwin's finches, we still lack a complete view of the feedbacks at play (Reznick 2016; Reznick et al. 2019). No study to date on these systems has attempted to describe feedbacks in an integrated and consistent manner, by inferring effects between all relevant ecological, evolutionary, and environmental variables in a consistent statistical/mathematical framework. The complexity of the pathways and the potential importance of indirect and interactive effects means that eco-evolutionary feedbacks cannot be understood from studying pairwise interactions between variables (Duckworth and Aguillon 2015; TerHorst

et al. 2018). Mortensen and colleagues provided a complete mapping of the interplay between phenotypic change (timing of egg laying of waders), ecological change (e.g. plant flowering), and environmental change (timing of snowmelt) (Mortensen et al. 2016). Although they demonstrated the usefulness of integrated approaches, such as structural equation modelling, they did not establish the evolutionary nature of the change in the phenotype, preventing us from making inference about the structure of the evolutionary process at play in the system. There is a need for similar approaches in systems where fast evolution is known to be at play.

This lack of quantitative evidence prevents us from answering key questions about eco-evolutionary dynamics in nature. (1) We still do not know the importance of direct and indirect effects linking ecological and evolutionary change, especially compared to environmental effects (Brunner et al. 2019; De Meester et al. 2019; Hendry 2019). (2) We do not know whether these effects are consistent in time, or if they are highly variable, due to context-dependence (Brunner et al. 2019). (3) We do not know to which extent these effects vary across similar traits and species (Brunner et al. 2019; De Meester et al. 2019; Hendry 2019). (4) Ultimately, this prevents us from assessing the ubiquity and repeatability of feedbacks in nature (Schoener 2011; Ellner 2013; Luo and Koelle 2013; Koch et al. 2014; Rodríguez-Verdugo, Buckley, and Stapley 2017).

1.4 Quantifying feedbacks

There is no consensus regarding methods for quantifying eco-evolutionary feedbacks in real systems. The main theoretical framework to study feedbacks consists of Ordinary Differential Equa-

tion (ODE) systems (Yamamichi and Ellner 2016; Patel, Cortez, and Schreiber 2018). These models broadly rely on combining the Price equation, or a similar fitness gradient-based equation, to model changes in phenotype, and a Lotka-Volterra system to model ecological change (e.g. Day and Gandon 2006; Day and Gandon 2007; Ellner, Geber, and Hairston 2011; Van Velzen and Gaedke 2017; Patel, Cortez, and Schreiber 2018). In these models, feedbacks are characterised by looking at the Jacobian matrix of the system (Patel, Cortez, and Schreiber 2018). The Jacobian matrix contains the sensitivity of evolutionary change to a change in the ecological state, and vice versa. More complex models, such as integral projection models (IPMs) (Coulson et al. 2015; Childs, Sheldon, and Rees 2016), or individual- and agent-based models (IBMs, ABMs) (e.g. Okamoto and Amarasekare 2017), allow for more realism in the ecological and genetic structure of populations. In these models, feedbacks can be tested through simulation and virtual experiments (e.g. Bonte and Bafort 2019).

The main difficulty in quantifying eco-evolutionary feedbacks with mechanistic models comes from the complexity of the underlying mechanisms (Koch et al. 2014). For instance, if we were to model the eco-evolutionary dynamics of a population, considering a single trait in a basic ecosystem featuring a resource and an abiotic environmental variable, we would need to define 16 processes to describe the interactions between these variables. In most cases we lack a suitable mechanistic representation for these processes (Jost and Ellner 2000). This means that feedback effects quantified to date may be biased by the mechanistic structure chosen to represent them. The second limitation of this approach is that these models are cumbersome, and hence rarely confronted to

time series data from a real system. In spite of a few attempts at parametrising them with data from real systems (e.g. Childs, Sheldon, and Rees 2016; Bruijning, Jongejans, and Turcotte 2019; Cortez, Patel, and Schreiber 2020), and recent studies advocating the use of theoretico-empirical approaches (Rosenbaum et al. 2019; Pontarp, Brännström, and Petchey 2019), their potential for quantifying eco-evolutionary feedback in real systems remains underused.

In parallel to this mechanistic approach, empirical studies relied on statistical models to infer eco-evo and evo-eco effects from time series data. Hairston and colleagues developed a statistical method, called the Geber method, to quantify the contribution of evolutionary change, namely heritable changes in the phenotype, to the population growth rate (Hairston et al. 2005). The method requires two steps: (1) to recover the effects of ecological, environmental, and evolutionary variables on the per-capita growth rate of the population via linear regression, and then (2) to compute the contribution of each variables to changes in the growth rate of the population via the chain rule. Hairston and colleagues applied the method to the medium ground finch population on Daphne Major island to quantify the contribution of changes in beak morphology to changes in the population growth rate (Hairston et al. 2005). They showed that the impact of phenotypic change on the population growth rate could be as important as that of ecological variables (e.g. seed availability). Though the method was used mainly to quantify the contribution of evolution to ecology (e.g. Ezard, Côté, and Pelletier 2009; Ellner, Geber, and Hairston 2011; Becks et al. 2012; Pigeon et al. 2017), it was also proposed as a method to quantify the contribution of ecological change to the dynamics of traits (Benthem et al. 2017). In spite of that, no study to our knowledge has

applied the Geber method in a bidirectional manner, to quantify the contribution of evolutionary change to ecological change, and vice versa. Furthermore, the simple linear models used to quantify the relationship between the growth rate of the population and the state of the system often ignore potential non-linearities in the processes stemming from context-dependence in effects. It is hence often unclear to which extent the feedback effect size reported may be contingent on the model structure chosen in the study (Adamson and Morozov 2013), and whether these structures are appropriate representations of feedback mechanisms. There have been attempts at embedding the Geber method in more mechanistic models, to portray more faithfully the potential feedbacks at play (Ellner, Geber, and Hairston 2011; Van Velzen and Gaedke 2017). For instance, the method was refined by Ellner to separate the contribution of adaptive changes from plastic changes, by modelling the dynamics of the traits with the Price equation (Ellner, Geber, and Hairston 2011). In spite of these attempts, the empirical approach suffers from the same mechanistic pitfall as its theoretical counterpart.

1.5 Research aims

Overall, we lack quantitative evidence for eco-evolutionary feedbacks in natural systems with multiple species, traits, resources, in a changing environment. This stems from the complexity of the potential processes at play, and the lack of well-established specialised methods to infer effects between ecological and evolutionary variables. We hence see three main avenues for improving upon current methodologies, with the aim of inferring eco-evolutionary feedback effects from time series data collected in natural systems.

First, we need to merge empirical and theoretical approaches for quantifying feedbacks (Luo and Koelle 2013; Lion et al. 2018). In particular, there is a clear benefit of combining models that properly account for the complexity of eco-evolutionary dynamics, with the Geber method, which allows to quantify the coupling between ecological and evolutionary change. The only attempt to our knowledge was a study by Van Velzen and colleagues, where they used the Geber method to quantify the coupling between the equations describing the ecological and evolutionary dynamics of a prey and its predator (Van Velzen and Gaedke 2017). The work however was theoretical, and was not applied to study eco-evolutionary feedbacks in a real system.

Second, we need to better account for the uncertainty in the mechanisms that underlie feedbacks, in order to assess more reliably their actual effect size. It can be challenging to prove that the eco-evolutionary processes are well represented by the equations used. This requires extensive model selection on a selected set of hypotheses. Even in this case, there is no guarantee that the set of hypotheses identified is suitable to describe the processes (Jost and Ellner 2000; Adamson and Morozov 2013). This problem does not arise in non-parametric models, where the mathematical structure of the processes is not specified (Jost and Ellner 2000; Wood 2001; Bonsall, Van Der Meijden, and Crawley 2003; Wu, Fukuhara, and Takeda 2005). Non-parametric models would hence be suitable to handle the uncertainty surrounding the mechanisms underlying eco-evolutionary dynamics. They would provide estimates for feedback effects that are not contingent on the mathematical structure chosen to model them.

Finally, we need to embed the quantification of feedbacks in a consistent Bayesian framework. So

far, most studies quantifying eco-evo and evo-eco effects have reported effect sizes (e.g. Hairston et al. 2005; Becks et al. 2012). The quantification of uncertainty received less attention (Benthem et al. 2017; Hendry 2019). There are more and more studies advocating the use of Bayesian methods for fitting dynamical systems in ecology and evolution (e.g. Fussmann et al. 2017; Rosenbaum et al. 2019; Pontarp, Brännström, and Petchey 2019). These methods would allow us to infer distributions for the effects involved in eco-evolutionary feedacks that are most likely given the time series data at hand. These techniques would hence provide a more thorough assessment of the uncertainty surrounding these effects (Pontarp, Brännström, and Petchey 2019).

1.6 NODEs

We propose that these three avenues can be addressed with the framework of Neural Ordinary Differential Equations (NODEs). A NODE can be viewed as a class of ODE that is partly or fully defined by an Artificial Neural Network (ANN) (Funahashi and Nakamura 1993; Chen et al. 2019). ANNs are non-parametric functions which approximate continuous functions up to a desired degree of precision. NODEs are hence capable of approximating any dynamical function non-parametrically (Chen and Chen 1993; Funahashi and Nakamura 1993).

They were first introduced by Funahashi in 1993 as a continuous equivalent of Recurrent Neural Network (RNNs) (Funahashi and Nakamura 1993). NODEs were mainly used to approximate the solution of ODEs (Meade and Fernandez 1994b; Meade and Fernandez 1994a; Jin, Nikiforuk, and Gupta 1995; Li, Ho, and Chow 2005), with applications in mathematical physics to solve

Partial Differential Equations (PDEs) (e.g. Aarts and Van Der Veer 2001). One would use the ANN to approximate the solution of the ODEs or PDEs as non-parametric functions of time. The ANN would then be trained to satisfy the equations of the system, at which point it would have converged to a satisfactory solution. This was a computationally friendly alternative to solving the system numerically.

These models were similar to partially specified models, introduced in Biology in the early 2000s (Jost and Ellner 2000; Wood 2001; Ellner, Seifu, and Smith 2002; Ramsay et al. 2007). Partially specified models relied on splines to approximate vital rate functions in ODE models as a function of age (Nisbet et al. 2004), population or predator density (Jost and Ellner 2000; Ellner, Seifu, and Smith 2002; Moe, Stenseth, and Smith 2002; Moe et al. 2005), or abiotic variables (Pasquali and Soresina 2018). For instance, Jost and Ellner used splines to learn non-parametrically the functional response of the prey to population and predator density (Jost and Ellner 2000). Although viewed as promising (Bjørnstad and Grenfell 2001), the framework is still rarely used, probably in line with a burdensome and computationally intensive implementation.

More recently, NODEs and NPDEs have gained traction across a range of fields. NODEs have resurfaced in the field of Artificial Intelligence (AI) as an alternative to RNNs (Chen et al. 2019; Rackauckas et al. 2019; Rubanova, Chen, and Duvenaud 2019; Massaroli et al. 2020). NPDEs are increasingly used in computational physics to approximate governing equations where theory is missing (Raissi, Perdikaris, and Karniadakis 2019; Berg and Nyström 2019), in particular in hydraulics (Sinchev et al. 2018). They have also been used in neuroscience as a mechanistic model

to represent the behaviour of motoneurones in an Ape (Sussillo et al. 2015).

NODEs have not been formally applied in an ecological and evolutionary context. There is only one study to our knowledge that used NODEs to model prey-predator dynamics in a chemostat system (Wu, Fukuhara, and Takeda 2005). Their modelling framework was disconnected from the rest of the literature as they did not label their model as a NODE system. Yet their study showed promising results, as the ANN embedded in the ODE system was able to approximate the functional response of the study species to its resource.

There is a huge potential for NODEs to further our understanding of eco-evolutionary dynamics. Their main strength lies in the fact that they do not require a prior understanding of the mechanisms underlying the dynamics to appropriately model the system. This is because the ANNs embedded in the ODE skeleton of NODEs can be trained to approximate non-parametrically the processes that drive change in the variables of the system from time series data. They would hence allow us to infer the strength of the coupling between ecological and evolutionary variables even where we do not know of a suitable mathematical form to describe them.

1.7 Chapter overview

In this thesis, we hence propose to explore the potential of NODEs to infer eco-evolutionary feedbacks in time series collected in natural systems. In particular, we use NODEs to recover the drivers of ecological and evolutionary change in a system with multiple species and traits under environmental change.

In the first chapter we establish the NODE framework to study ecological and evolutionary dynamics. We describe the mathematical foundation of NODEs and how they can be used to model change in ecological and evolutionary variables. We explain how to recover biological insights from them, such as the effect (sensitivity) and contribution (namely the product of the effect and of the dynamics) of the variables of the system on the population growth rate and phenotype dynamics. We apply NODEs to study the ecological interaction between hares and lynx in the famous prey-predator time series provided by Odum and Barrett (Odum and Barrett 1972). We conclude by giving guidelines for applying NODEs to a wide range of biological systems.

In the second chapter we provide an application of NODEs to studying ecological interactions in three replicates of a chemostat prey-predator system. The aim of this study is to provide a more concrete example of a NODE implementation to study the consistency of the dynamics in real ecological system, before diving into eco-evolutionary dynamics. We find that dynamics and dynamical processes (ecological interactions) vary substantially across systems that have been designed as experimental replicates. This demonstrates the variability of ecological dynamics and shows the viability of NODE systems in characterising ecological dynamics in a real biological system.

In the third chapter, we apply NODEs to study eco-evolutionary feedbacks in Darwin's finches on Daphne Major island. We infer the strength of the coupling between phenotypic and ecological change in the finch population and in their resource (seeds). We address the consistency of these effects in time, characterise the main pathways for interplay between ecological and evolution-

ary change, and how these vary across traits and across the two closely related species of finch present on the island. We conclude by comparing our findings to the current state of the knowledge regarding feedback effects at play in this system.

In the final chapter, we discuss our findings across the three previous chapters. In particular, we discuss how differences in dynamics may arise in two highly similar systems, leveraging the variability of dynamics found in the microcosm replicates, and the differences in feedback structure found in Darwin's finches. We also discuss the usefulness of NODEs in studying eco-evolutionary dynamics, highlighting the great benefit of bypassing the need for a mechanistic understanding of the processes at play. We conclude by providing avenues for future investigations in eco-evolutionary dynamics using NDE systems. These include merging NODEs with the Price equation to get estimates of fitness gradients and selection on the phenotype. Or by extending NODEs into NPDEs or Neural Integral Projection Models to study the eco-evolutionary dynamics of continuously and discretely structured populations.

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Part II

Chapter 2: Neural ordinary differential equations for ecological and evolutionary time series analysis

Neural ordinary differential equations for ecological and evolutionary time series analysis

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Abstract

1. Inferring the functional shape of ecological and evolutionary processes from time series data can be challenging because processes are often not describable with simple equations. The dynamical coupling between variables in time series further complicates the identification of equations through model selection as the inference of a given process is contingent on the accurate depiction of all other processes. 2. We present a novel method, neural ordinary differential equations (NODEs), for learning ecological and evolutionary processes from time series data by modelling dynamical systems as ordinary differential equations (ODEs) and dynamical functions with artificial neural networks (ANNs). Upon successful training, the ANNs converge to functional shapes that best describe the biological processes underlying the dynamics observed, in a way that is robust to mathematical misspecifications of the dynamical model. 3. We demonstrate NODEs in a population dynamics context and show how they can be used to infer ecological interactions, dynamical causation, and equilibrium points. We tested NODEs by analysing well understood hare and lynx time series data, which revealed that prey-predator oscillations were mainly driven by the inter-specific interaction, as well as intra-specific density-dependence, and characterised by a single equilibrium point at the center of the oscillation. 4. Our approach is applicable to any system that can be modelled with differential equations, and particularly suitable for linking ecological, evolutionary, and environmental dynamics where parametric approaches are too challenging to implement, opening new avenues for theoretical and empirical investigations.

1 Introduction

Understanding and predicting dynamics is at the heart ecology and evolution, whether it is to forecast the outcome of evolutionary responses (Norberg et al. 2012), adverse consequences of climate change (Cotto et al. 2017), or to assess population viability (Pierson et al. 2015). The complexity of biological systems hinders our ability to anticipate how they change. For instance, even a seemingly simple system of two interacting species like the hare-lynx system can lead to intriguing and unpredictable dynamics, such as hares apparently feeding on lynx (Deng 2018). While incorrectly inferring the drivers of historical hare and lynx population dynamics might have limited consequences, incorrect predictions of environmental threats, such as effects of pests on crops, harvesting of natural resources, or epidemics (e.g. Ferguson et al. 2020), may have a greater societal impact. It is hence paramount that we continue improving our capacity to understand and forecast the dynamics of natural systems.

In practice, gaining both understanding and predictability of a given system can be achieved through dynamical modelling of time series data. The general idea is to formulate a mathematical model that describes changes in the key variables of a given biological system, and to constrain it to behave like the real system via model fitting. The analysis of the dynamical properties of the model then reveal key biological properties of the biological system such as ecological interactions (e.g. Hiltunen et al. 2013), dynamical causation (Sugihara et al. 2012), equilibrium points and stability (e.g. Cortez and Patel 2017). Dynamical system modelling is broadly divided into parametric and non-parametric dynamical models, depending on the nature of the functions that determine the

dynamics of the key variables.

Parametric dynamical models broadly consist of time difference equation systems in discrete time, such as auto-regressive models (e.g. Stenseth et al. 2002), and ordinary differential equation systems (ODEs) in continuous time (e.g. Deng 2018). The general approach consists in translating hypotheses regarding the dynamics of the system variables into a parametric mathematical model, and then finding parameters that produce dynamics consistent behaviour of the system. This approach is limited by our capacity to formulate assumptions and conceptualise the system, which makes it challenging to build a suitable model for a given ecological system, and can be problematic in cases where fast action is required (e.g. dealing with invasive species, or algal blooms).

The counterpart of parametric dynamical models are non-parametric dynamical models, primarily consisting of recurrent neural networks (RNNs, e.g. Lek and Gue 1999). In practice, RNNs are fitted to the time series by predicting iteratively the state of the system at the next time step given the current state and associated covariates. These models have been applied successfully to study ecological dynamics, such as the growth of pine trees (Chon et al. 2000), changes in aquatic benthic communities (Chon et al. 2001), and the dispersal of ungulates (Dalziel, Morales, and Fryxell 2008). The main disadvantage of these approaches is that they are not embedded in a theoretical framework and thus provide limited insights into the mechanisms at play.

Neural ordinary differential equations (NODEs), a recent breakthrough in AI research (Chen et al. 2019; Rubanova, Chen, and Duvenaud 2019), offer a promising alternative, as they combine the strengths of both parametric and non-parametric approaches to time series analysis. NODEs are de-

fined by embedding artificial neural networks (ANNs), which are universal function approximators (Chen and Chen 1993), in ODE systems, which are powerful mathematical models for dynamical systems, allowing ANNs to approximate key dynamical processes (i.e. functional representations describing how the state variables affect each other and determine the dynamics of the system) (Chen et al. 2019; Rubanova, Chen, and Duvenaud 2019). Then by training the NODE system to replicate time series of observations of the system state, the ANNs converge to the functional shapes that best describe the underlying dynamical processes (e.g. Wu, Fukuhara, and Takeda 2005). NODEs hence provide a novel way to infer hidden dynamical processes from time series data (Chen et al. 2019; Rubanova, Chen, and Duvenaud 2019), as hypotheses can be specified with parametric ordinary differential equations, and unknown processes can be approximated non-parametrically by the ANNs (e.g. Wu, Fukuhara, and Takeda 2005).

Hybrid approaches combining ANNs and ODEs have been applied with success in the past across a range of fields. For example, physicists have recently applied approaches combining partial differential equations (PDEs) and ANNs to model fluid dynamics (Sinchev et al. 2018), and to discover governing physical equations from data (Berg and Nyström 2019). Neuroscientists have modelled the activation dynamics of interacting populations of neurones in an Ape with a NODE-like system, faithfully reproducing the behaviour of motoneurones (Sussillo et al. 2015). Only one study in ecology, to our knowledge, successfully combined ANNs with ODEs to learn functional responses in a prey-predator system, reproducing intriguing non-stationary oscillations (Wu, Fukuhara, and Takeda 2005).

It is our view that the potential of NODEs to further our understanding of ecological and evolutionary system dynamics remains largely unexplored, as no study to date has formally introduced the method in an ecological dynamics context and demonstrated which, and how, biological insights could be derived from applying them to real ecological data. For instance, NODEs could be used to learn ecological interactions from time series data, establish dynamical causality between system variables, and determine equilibrium points in a community dynamics context. In doing so NODEs are not contingent on assumptions and hence offer interesting counterbalance points to results obtained from parametric dynamical models.

Our aim in this manuscript is to introduce the NODE framework and demonstrate how it can be applied to real ecological data, with a focus on learning ecological interactions, dynamical causality, and equilibrium points. To do this we define the mathematical pre-requisites and general steps to implement NODE systems for a given time series. Then, we demonstrate how the approach can be used in practice by analysing the dynamics of a di-trophic system, the hare-lynx pelt count time series (Odum and Barrett 1972). In particular, we highlight how ANNs uncover the shape, direction, and strength of ecological interactions in the time series, as well as dynamical causality and potential equilibrium points. Finally, we discuss these results in light of the biology of the system and highlight further applications and developments of the framework in the context of ecological and evolutionary dynamics.

2 Material and Methods

2.1 Method overview

The following sections describe how to define, train, and analyse a NODE system in a population dynamics context (an overview is presented in Fig. 1). In particular, we use NODEs to recover non-parametric approximations of the per-capita growth rate of the different species present in a community, from time-series data. From these non-parametric approximations, we demonstrate how to recover the direction and strength of species interactions, the contribution of each species dynamics to the dynamics of other species, as well as equilibrium points in the state space of the system. We have chosen to demonstrate the method in a population dynamics context as it is a subject of interest to many ecologists, and makes the workings of the method more concrete and accessible. Throughout the following sections, we encourage the reader to keep in mind that NODEs can be used to model the dynamics of other biological variables, beyond population density, such as phenotypic trait and spatial dynamics, amongst others, making it an extremely versatile method. These other applications are described in the discussion.

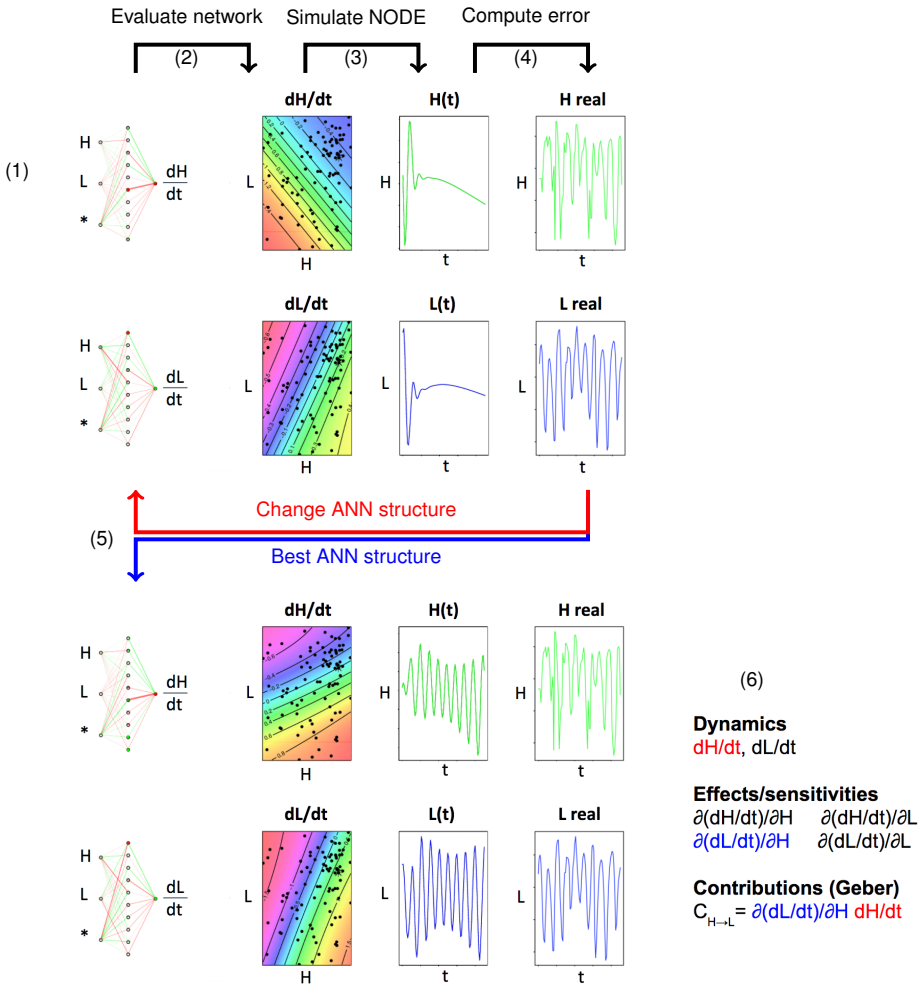

Figure 1: Overview of training and analysis of NODE systems. (1) The dynamics of the state variables are defined as neural networks with inputs being the state of the system (e.g. hare H, lynx L, other variables $\star$). (2) This imposes a shape for the dynamics of each population as a function of the state of the system. (3) The model can be simulated like any regular ODE to generate predicted time series for the system states. (4) The predictions are compared to observed states assuming an error model (in the present study a Bayesian model). (5) The error is minimised by repeating steps (1) to (4) with different network parameters, at which point the networks will have converged to the shapes that best describe the observed dynamics. (6) Finally, the best NODE system can be analysed to explore state-dependence in dynamics (effects), dynamical coupling (contributions), and more.

2.2 Defining NODEs

For the sake of simplicity, we consider extending simple ODE population dynamics models into NODE population dynamics models. To start with we define several key elements of simple ODE population dynamics models: let X denote the density of species X, let r_x denote the per-capita growth rate of species X. The dynamics of X in continuous time can then be written as a simple differential equation $dX/dt = r_x X$. The dynamics of any other species Y, for instance a predator of X, can be written as $dY/dt = r_y Y$. Traditionally, we would define per-capita growth rates as parametric equations, based on our biological knowledge of the drivers of the changes in the density of these populations. For instance, the Lotka-Volterra model assumes a linear decrease in the growth rate of the prey with predator density, $r_x = a - bY$, and a linear increasing function of prey density for the per-capita growth rate of the predator, namely $r_y = cX - d$. This parametric construction captures the direction of the ecological interaction between the two species, which in this case is a trophic interaction benefiting the lynx. The actual direction and strength of the interaction can be obtained by estimating the parameters a, b, c, and d from time series data by fitting the ODE system to the time series of population densities (e.g. Kendall et al. 2005; Demyanov, Wood, and Kedwards 2006; Fussmann et al. 2017).

The benefit of this approach is that it embeds the ODE population dynamics model in the real world by providing parameters that are consistent with the dynamics of the real system. The issue with this approach is that the values of the parameters, and therefore of the direction and strength of the ecological interaction, are contingent on the choice of mathematical function for the growth

rates. In practice, due to the complexity of the processes that underlie the per-capita growth rates of species, we have a low chance of choosing an appropriate mathematical form. Furthermore, because all variables are coupled dynamically, misspecifying the per-capita growth rate in a single species will impact the dynamics of all others, and potentially bias the inference of all species per-capita growth rates. While it is feasible to test different mathematical functions through model selection in a low dimensional system, it becomes rapidly infeasible in larger systems. For instance, a three species population dynamics model features 9 possible pairwise interactions (i.e. density-dependencies in per-capita growth rates), so that even simply testing for the absence or presence of each interaction requires model selection in a model space of size 81.

This is why we propose to use a NODE system instead (or in addition to the parametric approach). A NODE is a class of ODE in which some functions are inferred non-parametrically with artificial neural networks (ANNs), rather than parametrically. ANNs should not be viewed as anything more than flexible functions of biological variables (e.g. species density) that can produce any continuous shape, and which can describe any biological quantity (e.g. per-capita growth rates). Therefore, while fitting a parametric ODE model provides estimates of parameters, fitting a NODE model provides estimates of entire functions. And instead of looking at specific parameter values, biological processes are studied by looking at the shape of the non-parametric functions, and dynamical behaviour they enforce. The benefit of this approach is that the inference of biological functions that underlie the dynamics of the system, such as per-capita growth rates, as well as any inference derived from them, are not contingent on our assumptions or on the mathematical

functions we might have chosen to portray them.

More particularly in the case of population dynamics, we can turn the simple ODE population dynamics model that we have developed so far into a NODE system by defining the per-capita growth rate of the populations as non-parametric functions of the species densities, instead of a parametric one, more formally, $r_x = s(X,Y)$, where s is a non-parametric function of the density of species X and Y. The dynamical equations for species X and Y thus become

$$\begin{aligned} \frac{dX}{dt} &= s1(X,Y)X \\ \frac{dY}{dt} &= s2(X,Y)Y \end{aligned} \tag{1}$$

where $s1$ and $s2$ denote the fact that the per-capita growth rates of X and Y are determined by two independent non-parametric functions s. The only biological assumption that needs to be made upon defining a NODE system to infer per-capita growth rates are the dependences of the growth rates of the species on the other states of the system. For instance, the construction $r_x = s(X)$ would imply that the per-capita growth rate r_x may only be subjected to intraspecific density-dependence, and may not be affected by changes in the density of species Y. In practice, this can be done simply by specifying manually which variables should be considered as inputs in the non parametric functions s.

The second step is to define the properties of the non-parametric functions s, that is the specifications of the ANNs. In this paper we consider a specific class of ANNs, called single layer perceptrons (SLPs), which is a widespread and mathematically convenient choice due to their sim-

plicity (e.g. Funahashi and Nakamura 1993; Aarts and Van Der Veer 2001; Wu, Fukuhara, and Takeda 2005; Mai, Shattuck, and O'Hern 2016; Sinchev et al. 2018). They are the most simple form of ANNs as they correspond to a weighted sum of basis functions f, more formally

$$\begin{aligned} s(X,Y,...) = \beta_0 + \beta_1 f(\beta_{10} + \beta_{11}X + \beta_{12}Y + ...) + \\ \beta_2 f(\beta_{20} + \beta_{21}X + \beta_{22}Y + ...) + ... + \\ \beta_i f(\beta_{i0} + \beta_{i1}X + \beta_{i2}Y + ...), \end{aligned} \tag{2}$$

where the β_{ij} are the parameters of the network.

The first key element of the networks that we need to define are the basis functions f. There is strong incentive for using sigmoid basis function given that the capacity of SLPs with sigmoid basis function to reproduce the shape of any continuous function has been established theoretically (Chen and Chen 1993). This property has been extended to NODEs relying on SLPs with sigmoid basis functions which have been shown to be able to reproduce the behaviour of any dynamical system with continuously defined differential operators (Funahashi and Nakamura 1993). In practice, however, certain basis functions are better at producing specific shapes. For instance, gaussian functions are suitable for producing gaussian-like shapes, with multiple peaks and valleys, which may be easier to train if the phase space is thought to be bell-shaped. The identity basis functions simplify the SLPs back to a linear model. In a population dynamics context, this implies that there are no context-dependence (or non-linearities) in the pairwise interactions between species. It is hence possible to test the robustness of the results to the implementation of context-dependence in

the effects of variables by switching the basis function from sigmoid to identity.

The second and final network element that needs to be specified is the number of intermediate nodes, namely the number of times the basis functions are summed in equation (2). There is a strong theoretical grounding for choosing a number of nodes that is at least twice as large as the number of input variables in the network to ensure that any continuous shape can be produced by the neural network (Chen and Chen 1993). For instance, if we modelled the per-capita growth rate of the lynx r_y as a function of hare and lynx density X and Y, namely $r_y = s(X,Y)$, we would need at least $n = 4$ nodes in the network. In practice, this number should also be as low as possible as it would otherwise complicate the training of the neural network (e.g. Wu, Fukuhara, and Takeda 2005). It is common practice to use 10 nodes, which is suitable for small ODE systems (e.g. Wu, Fukuhara, and Takeda 2005). In practice, there is no need to manipulate the number of nodes to change the complexity of the shape of the network as this is handled by the parameters of the networks.

2.3 NODE fitting

Fitting NODE systems to time series involves the same steps that are required for ODE systems, namely defining and optimising an error function. However, they require a couple of extra steps to account for the fact that NODEs are prone to overfitting and getting trapped in local maxima, due to being larger than parametric ODEs by at least an order of magnitude.

The first step is to define a simple Bayesian model to compute the posterior probability density of

the population density predicted by the NODE system given the population densities in the time series, which can be written as $p(X,Y|x,y) \propto p(x,y|X,Y)p(\beta)$, where x and y are the observed population densities, X and Y the population densities predicted by the NODE system, obtained by simulating the NODE system with an ODE solver, and β are the parameters of the neural networks. For the sake of simplicity, we assume normal distributions for the residuals of model predictions with a dispersion parameter σ_1 that we use to control the precision of the fit, more formally, $e_t \sim \mathcal{N}(0, \sigma_1^2)$, iid. Given the flexibility of these models we treat the dispersion σ_1 as *known* to dictate how closely the model should fit the data and therefore reduce the chance of overfitting. In addition, we define normal prior distributions for the parameters of the network with a mean of 0 and dispersion σ_2 that we use to control the complexity of the network, $\beta_{ij} \sim \mathcal{N}(0, \sigma_2)$, iid. The idea is that low values of dispersion σ_2 constrain the parameters of the networks to be close to 0, which also constrains the shape of the neural network to be simple and linear. In contrast, increasing the dispersion of network parameters allows for more complex, nonlinear shapes for the network. This provides a way of limiting the risk of overfitting, while assessing the robustness of results and dynamics to increasing levels of complexity/nonlinearity in the shape of the population growth rates. One must choose carefully the dispersion parameter controlling the strength of parameter constraint, as too high levels of constraint may reduce the variance of the parameter, and bias mean estimates towards 0. It is hence important to assess the robustness of the results to the dispersion parameter.

The second step consists in fitting the NODE system, which can be done by finding the network

parameters (and thereby the shape of the functions) that maximise the posterior distribution. In this manuscript we rely on the BFGS gradient descent method to optimise the posterior distribution. There exist other techniques to fit these models which we discuss in the code implementation section.

The third and final step, which is not necessary if we are only interested in finding the best fit, is to quantify the uncertainty around the NODE predictions given the choice of the dispersion parameter for the likelihood and priors. In this manuscript we use a rejection sampling scheme of the posterior distribution to recover approximated posterior distributions of the network parameters (Gelman et al. 2013), and thereby of the shapes of the per-capita growth rate and biological quantities that we derive from them. Samples from the posterior distribution are generated by randomly drawing parameters according to a known probability distribution, centered around the best identified parameter vector, and discarded with a probability proportional to their posterior density (Gelman et al. 2013).

2.4 NODE analysis

Once the fitting of the NODE system to the time series is completed, we can analyse the model. The general NODE model that we have developed in the context of population dynamics returns non-parametric approximations of the per-capita growth rates of each species, as a function of the density of other species. Analysing the model comes down to analysing the per-capita growth rate functions of each species, and studying the dynamical behaviour that they impose, such as

oscillations and equilibrium points.

2.4.1 Inferring direction and strength of ecological interactions

Per-capita growth rate functions contain essential information regarding the ecological interactions between the species of the system. First, the direction of the interaction between the species can be approached by studying how its per-capita growth rate changes with the density of other species. This information is captured by the slope, or sensitivity, of the per-capita growth rate with respect to the density of each species, noted $\partial r_y/\partial X$ where r_y is the per-capita growth rate of species Y, and X is the density of species X. For instance, considering the hare-lynx system, $\partial r_l/\partial H = 0.5$ would mean that the per-capita growth rate of the lynx (r_l) increases by 0.5 per unit of hare density (H). In biological terms, this means that hare density tends to increase the per-capita growth rate of the lynx, and therefore that a higher prey density improves the predator population growth rate.

2.4.2 Dynamical coupling between variables

Computing effects alone is necessary but not sufficient to establish whether two variables are coupled dynamically, that is whether changes observed in one variable were caused by changes in the other. For example, the growth rate of a prey may be affected negatively by predator density, but the actual contribution of the predator population to the dynamics of the prey can either be positive, zero, or negative depending on whether predator density is decreasing, remaining constant, or increasing. In the first case, the prey population would grow as a result of the alleviation of predation pressure. It is thus important to consider contributions in addition to effects/sensitivities.

Contributions of the species X to the dynamics of any species Y can be computed following the Geber method (Hairston et al. 2005), which amounts to multiplying the dynamics of X by the effect of X on the growth rate of Y, more formally $C : X \rightarrow Y = dX/dt \times \partial r_y/\partial X$. The total contribution of a variable over a time period can be computed by summing the absolute value of its contribution at each time step across all time steps. This value gives an idea of how important a given variable is for the dynamics of the focal population.

2.4.3 Finding equilibrium points

In addition to effects and contributions, it is also possible to derive equilibrium points from the analysis of the non-parametric approximations of the population growth rates. Equilibrium points correspond to points in state space (i.e. particular combinations of population densities) at which the growth rate of the populations are null. Equilibrium points can be found numerically by evaluating the dynamics of the system for different combinations of population densities, just like any regular non-analytically tractable ODE systems. This last application of NODEs can prove particularly useful for managing natural populations, as equilibrium points found are not subjected to potential misspecifications of the mathematical structure of the model.

2.5 Code implementation

There are two well-established and tested repositories for NODEs in Python (Chen et al. 2019) and Julia (Rackauckas et al. 2019). In both cases, the repositories provide state of the art fitting algorithms, such as the adjoint sensitivity method, and methods for analysing NODEs. However, these

repositories do not provide options for performing Bayesian inference, and there are no implementations directly available to recover the biological quantities of interest discussed in the previous section. We hence provide an R implementation of the NODE population dynamics models presented in the previous sections. It is our view that an R implementation would be more useful to many ecologists given the predominance of the R language in the field. Furthermore, we coded the repository with a focus on simplicity and clarity rather than computational efficiency to facilitate and encourage customisations of the method to pursue other biological aims beyond the ones presented here. The code is modular as well and can be applied to any time series, be it formatted as a table with time steps in the first column, and handles automatically the specifications of the networks and of the fitting.

The steps to implement a NODE for a given time series in the R language are as follows: (i) format and standardise the time series (TS.format function), (ii) create a NODE object list containing the dependence of each variable on the variables of the system (NODE.init function), (iii) define the dispersion parameters of the likelihood and prior functions σ_1 and σ_2 (function .error.normalBayesian), (iv) optimise the posterior distribution for a specified number of iterations and dispersion parameters, based on the *ode* function in the *odeSolve* package for simulation and *optim* function that performs BFGS gradient-descent optimisation, which is not as efficient as the fitting methods in the python and Julia repositories, but is still robust and commonly used for fitting ODEs and ANNs, (v) quantify uncertainty around model predictions through rejection sampling of the posterior distribution, which is an approximate Bayesian computational (ABC) method that

provides approximations of the error around model estimates (function .ABC), (vi) extract and visualise effects, contributions, equilibrium points with the various functions implemented in the repository.

The code is provided in full for the case study on a GitHub repository referenced in the data accessibility section. The implementation we provide also allows for the use a simple LASSO/ridge least square regression of the NODE system, in case the Bayesian implementation is deemed unnecessary. In addition to that, we provide supplementary files on the GitHub repository containing (1) a minimalistic implementation of a 2 variable NODE system, geared towards computational efficiency and fine customisation, as well as (2) an implementation of a 2 variable NODE system with a time-dependence embedded to model time-varying interactions between variables.

2.6 Case study: di-trophic prey-predator dynamics

System

In this section we provide an example of NODE implementation to study density-dependence in prey-predator cycles, using the well known hare-lynx system as a model (Krebs et al. 2006), thus facilitating the assessment of the consistency of our results with the literature. Hare and lynx display clear 10-year long population cycles, which are driven by a combination of phase dependence in predation and negative density-dependence in lynx (Slough and Mowat 1996; Stenseth et al. 2002; Krebs et al. 2006). Our aim is to use a NODE system to learn the per-capita growth rate of the prey and predator from time series of lynx and hare density. Then, by analysing the system,

we quantify intra- and inter-specific density-dependence in growth rates, and through the Geber method (Hairston et al. 2005), establish the respective contribution of intra- and inter-specific interactions to the demography of each population. The code, and additional explanations, can be found on a GitHub repository referenced in the data accessibility section.

We analyse a 90 year long time series of hare and lynx pelts (in tens of thousands), collected by trappers in the Hudson Bay area, from 1845 to 1935 (Fig. 4 first row, a. and b.), which displays characteristic oscillations, each lasting ten years on average (Odum and Barrett 1972). We chose this time series as it has been studied extensively, allowing for the most sensible comparisons between the results of our case study and the literature (Stenseth et al. 2002; Krebs et al. 2006).

Model specifications

We define a NODE system in which changes in hare and lynx densities are governed by a differential equation and their per-capita growth rate is approximated by an ANN

$$\begin{aligned} \frac{dH}{dt} &= r_H(H, L, \Omega_H)H \\ \frac{dL}{dt} &= r_L(H, L, \Omega_L)L \end{aligned} \tag{3}$$

where r_H and r_L denote the per-capita population growth rate of the hare and lynx population, as a function of hare and lynx density H and L, respectively, and Ω_H and Ω_L are the network parameters governing the shape of the growth rates. In practice, it is recommended to model the log of the density H and L for this allows to (1) write the model in a simpler form, namely $d(log(H))/dt = r_h$,

and $d(log(L))/dt = r_L$, (2) model the posterior distribution of the log density as a simple Bayesian model with a Gaussian likelihood, and (3) normalises the distribution of observed densities which facilitates the training of the SLPs.

The per-capita growth rates are approximated with SLP functions (equation (2))

$$\begin{aligned} r_H(H,L,\Omega_H) =& \beta_0 + \beta_1 f(\beta_{10} + \beta_{11}H + \beta_{12}L) + \\ & \beta_2 f(\beta_{20} + \beta_{21}H + \beta_{22}L) + ... + \\ & \beta_I f(\beta_{I0} + \beta_{I1}H + \beta_{I2}L),\ I = 10 \end{aligned} \tag{4}$$

of the hare and lynx densities H and L, weight vector Ω_H and Ω_L containing the network parameters β, and where the number of intermediate neurons is $I = 10$. The activation function is chosen to be sigmoid with form $f(x) = 1/(1+\exp(-x))$. The value of 10 hidden neurons was chosen by trial and error, it should be well over the dimension of the input (Chen and Chen 1993), but as low as possible (Wu, Fukuhara, and Takeda 2005).

Model fitting

The model was fitted to the time series following the approach described in the model fitting section of the methods (section 2.3). The fitting consisted in finding the parameters (and thereby the functional shape) for the non-parametric per-capita growth rates that maximise the posterior density of the population densities predicted by the dynamical system given the population densities observed in the time series and the prior distribution of the network parameters, more formally

$p(H,L|h,l) \propto p(h,l|H,L)p(\Omega)$. As stated before, low values for the dispersion parameter increases potentially the variance-mean bias in parameters. To account for this, we also compared model fits with different prior specifications, between $\sigma_2 = 0.1$ and $\sigma_2 = 0.3$, the former enforcing more simple linear functional shapes, the latter allowing for more complex non-linear relationships between the species. Finally, we did not perform cross validation of the model on a separate dataset, given that we were only interested in analysing effects within the time period considered. This, however, would be a requirement to guarantee the generalisability of model predictions and results outside of this time period.

Model analysis

Once this process was complete, the shape of non-parametric per-capita growth rates was analysed to determine the direction and strength of interactions between the two species, respective contribution of each species to the dynamics of the other, and candidate equilibrium points where both populations growth rates are 0. In particular, pairwise interactions between species was recovered by computing the sensitivity of the per-capita growth rates with respect to the other species density, for instance the effect of a change in hare density on the lynx growth rate was computed as Effect:$H \rightarrow L = \partial r_l / \partial H$. In turn, the contribution of the prey population dynamics to the dynamics of the predator population was computed by multiplying the dynamics of the prey population by its effect on the predator per-capita growth rate, Contribution:$H \rightarrow L = \partial r_L / \partial H \times dH/dt$ (Hairston et al. 2005). We computed the average effect of the prey population on predator dynamics by averaging the sensitivity of the predator per-capita growth rate across the entire time series. The

mean strength of the coupling between the dynamics of the prey and predator can be obtained by averaging the absolute value (or the square) of each pairwise contribution across the time series. Finally, we identified equilibrium points in the state space of the system by numerically solving the NODE system, that is finding H^* and L^* for which $dH/dt = dL/dt = 0$.

3 Results

3.1 Model fit

The fit of the best NODE system to the hare-lynx pelt count time series is presented in Figure 2. We were not able to obtain a fit for values of parameter prior dispersion below $\sigma_2 = 0.15$. The NODE system does well at capturing the main component of the 10-year oscillations and shows a slight trend for an increase in the amplitude of the oscillations towards the end of the time series. The fit yields a value of r-squared around 0.42, and the analysis of the residual autocorrelation demonstrates that the model does not capture faster oscillatory components of the dynamics (< 10 years). The increase in the prior dispersion parameter (up to 0.3), which enables greater non-linearity in the growth rates, did not improve the fit of the model. In addition, we find very narrow error bars around model predictions, estimated from rejection sampling, which means that estimated dynamics, effects, and contributions are highly identifiable for a given fit.

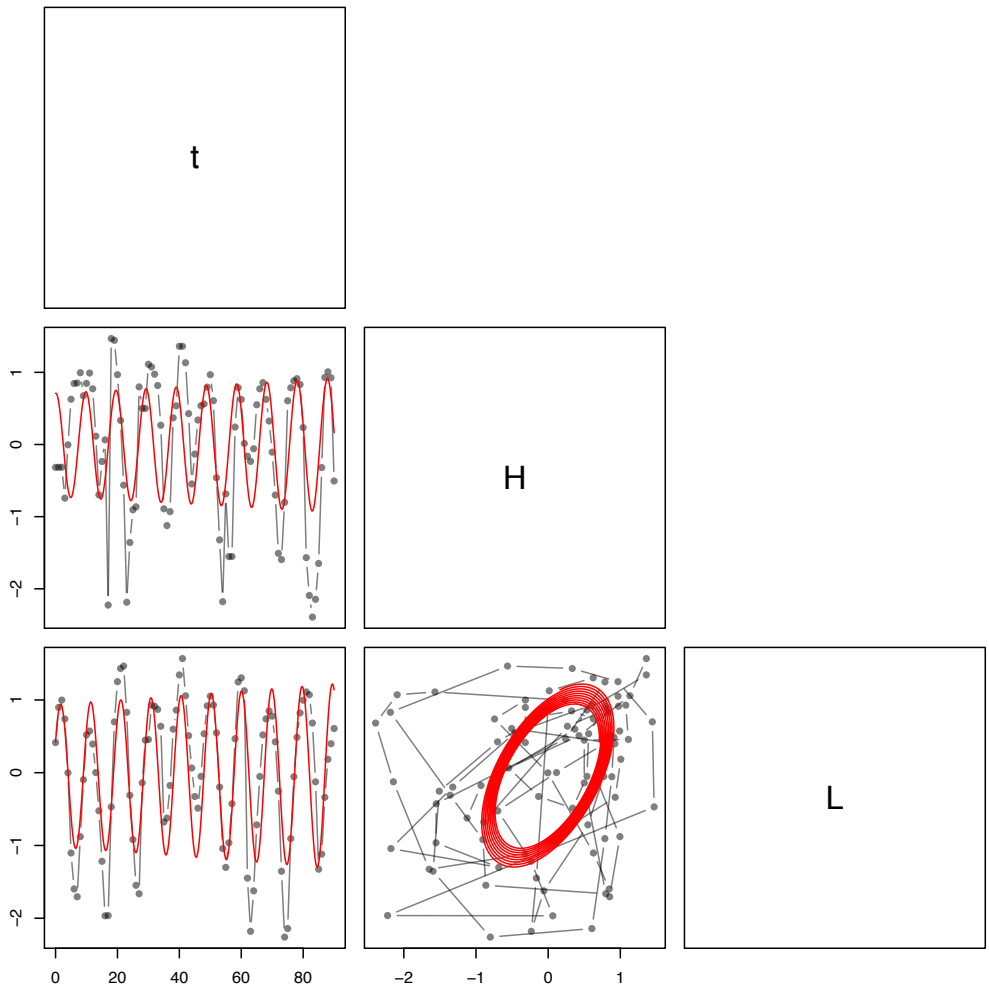

Figure 2: Fit of the hare-lynx NODE system to hare-lynx pelt count time series (Odum and Barrett 1972). The 3 state variables, that is time t, hare and lynx density H and L, are presented on the diagonal. The grey dots correspond to the number of either hare or lynx pelt counts reported for a given year. The red line corresponds to the number of pelt counts predicted by the best NODE system identified. The hare and lynx density were log transformed and standardised to prevent non real numbers for densities and improve fitting performance.

3.2 Dynamical interaction network and phase space

Figure 3 displays the shape of the hare and lynx growth rate (a. and b.) learned by the neural networks. These reveal a decrease in the hare growth rate with lynx density (Fig. 3 a.), and an increase with hare density, indicating positive intra-specific density-dependence. The lynx growth rate (Fig. 3 b.) increases with hare density and decreases with lynx density, indicating negative intra-specific density-dependence. Overall, there is no strong evidence of non-linearity in the shape of the growth rates. The combination of the two growth rate landscapes gives the combined phase space in figure 3 d. which reveal that the oscillations can be divided in four stages, where the two dominating stages correspond to areas where both populations are either growing, or declining (Fig. 3 d., red and blue area), which indicate tightly coupled oscillations. We found a unique equilibrium point in that system centered around the mean population densities (0 corresponds to the mean of the log densities). Overall, these results are consistent with a prey-predator interaction with negative density-dependence in the predator, and positive density-dependence in the prey (Fig. c.).

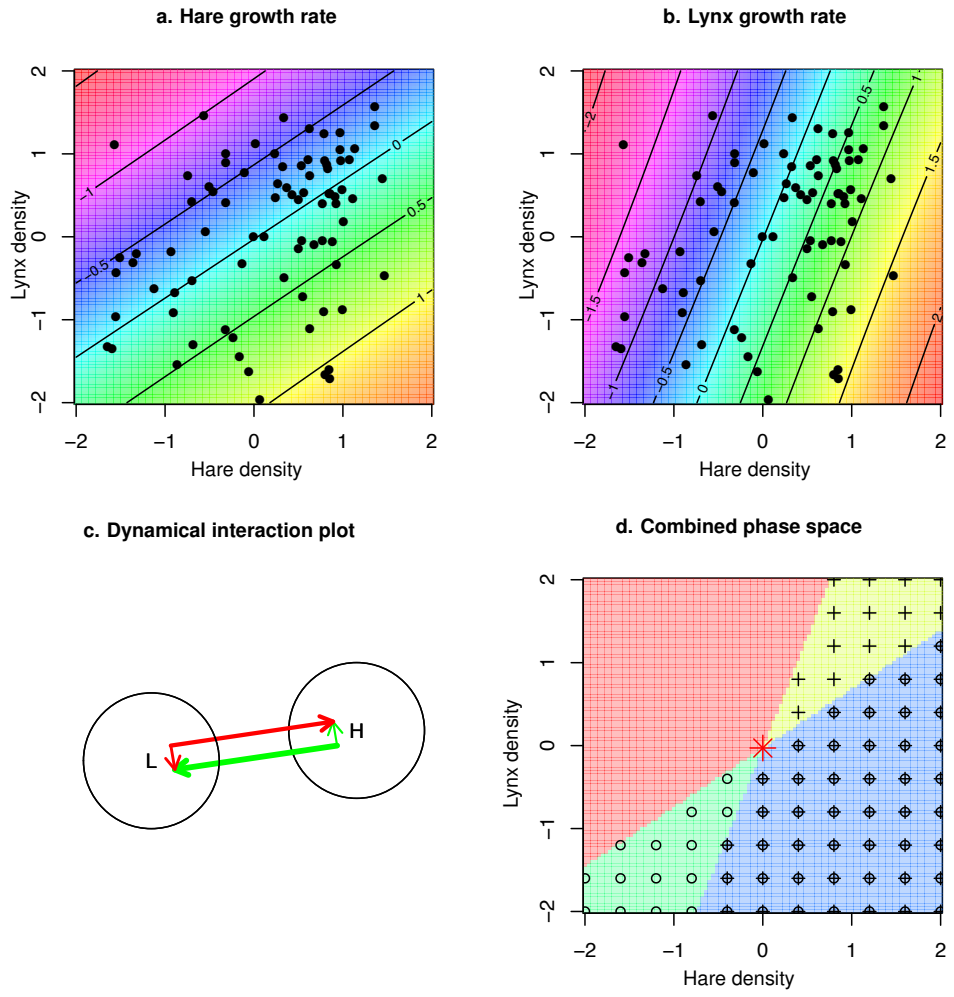

Figure 3: NODE approximation of the population growth rates. Graphs a. and b. correspond to the per-capita growth rates of the hare and lynx populations, respectively, as a function of hare and lynx density H and L. The black dots correspond to the data points in the time series. Cold colours (purple to blue) and contour lines below zero indicate areas where the populations are declining. Graph c. corresponds to the dynamical interaction network obtained by computing the sensitivity of each population growth rate to hare and lynx density, red and green arrows indicate negative and positive effects, respectively. Graph d. shows areas where both populations decline (red area), both grow (blue area, crossed circles), only the hare population grows (green area with empty dots), or only the lynx population grows (yellow area with crosses). The red star indicates the equilibrium point in the system (found by numerically solving the NODE system).

3.3 Effects and contributions

These results are further confirmed when dissecting the effects and contributions underlying the time series (Fig. 4). We find that the prey growth rate is affected positively by hare density and negatively by lynx density (Fig. 4 a. middle row). As for the lynx, we find a negative effect of lynx density on lynx growth, and a positive effect of hare density (Fig. 4 b. middle row). Overall, we find very limited variation of the effects throughout the time series (Fig. 4 a. and b. middle row). The contributions reveal that the main contribution to the dynamics of the prey is that of the predator (Fig. 4 a. last row), similarly the prey dynamics is the main contributor to the growth rate of the predator (Fig. 4 b. last row). This indicate that the inter-specific interaction is the main driver of the dynamics of both populations.

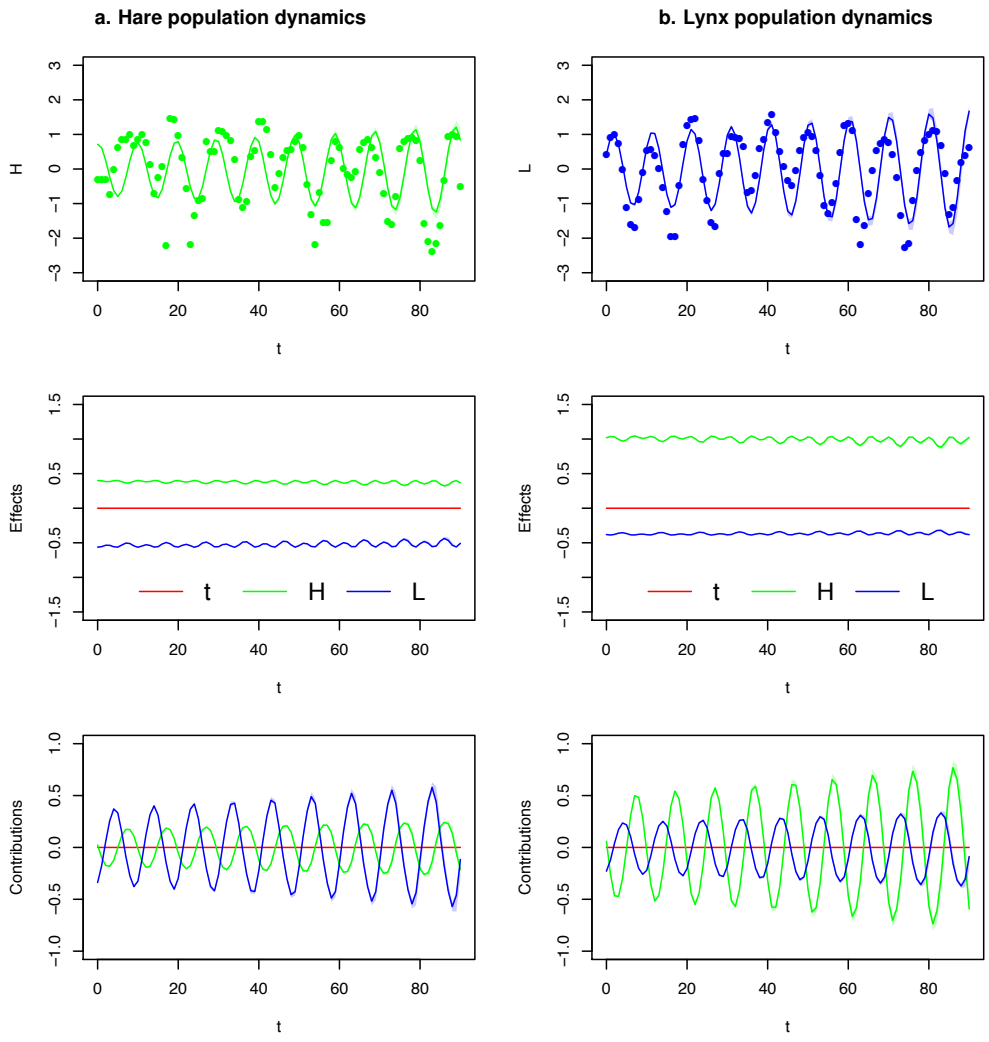

Figure 4: Effects and contributions derived from the NODE system fitted to the hare-lynx time series. Graphs on the first row correspond to hare (a.) and lynx (b.) population densities either observed (dots) or predicted by the best NODE system (solid line). Graphs on the second row display the effects/sensitivity of population growth rates to changes in hare and lynx density (i.e. the Jacobian elements of the networks in the NODE system). The graphs in the last row correspond to the contribution of these effects to hare and lynx population dynamics, respectively, computed by multiplying the dynamics of state variables (first row) with their effect (second row). In all graphs, the red lines indicate zero, and the shaded areas (very narrow) give the error around estimates derived from the model (light shading: 5-95%, dark shading: 25-75%, obtained from rejection sampling).

4 Discussion

The aim of this paper is to introduce the mathematical framework of Neural Ordinary Differential Equations (NODEs) to ecologists and evolutionary biologists and to illustrate how it can be used to learn ecological and evolutionary dynamical processes from time series data. We present the general framework and use it to identify the drivers of prey-predator oscillations. In particular, we infer per-capita growth rates in a time series of hare and lynx pelt counts from the Hudson Bay Company records (Odum and Barrett 1972). We were able to quantify precisely the intra- and inter-specific drivers of the dynamics of each population, revealing that the inter-specific interaction is the main driver of the oscillations, with no clear evidence for non-linearity in the relationship. These results demonstrate that the approach can provide valuable biological insights into the drivers of population dynamics, in a real setting. We discuss below the biological relevance of our results in light of the literature. We conclude by comparing this novel approach to existing methods for time series analysis, and highlight further applications to study ecological and evolutionary time series and connections with existing empirical and theoretical frameworks.

4.1 Hare-lynx case study

Overall, we find that the di-trophic NODE system considered in the present work fits reasonably well the hare-lynx pelt count time series, in spite of residual oscillatory components. We find that increasing the non-linearity of the hare and lynx growth did not improve the fit of the model, contrary to the general belief that neural networks can easily overfit. This strongly suggests that the

residual variation is attributable to state variables that are not modelled in the present system, such as climatic variables (Holyoak and Heath 2016), fluctuations in hunting pressures (Deng 2018), or age structure (Stenseth et al. 2002), and that increasing the complexity of the functional relationship between the hare and lynx population alone is insufficient to explain those residual dynamics. If nothing else, our study demonstrates that there seems to be a limit to the amount of variation that can be explained with di-trophic interactions as it accounts for up to 40% of the variation in the dynamics of the system, no matter how complicated the driving functions are.

We found that the inter-specific interaction was the main driver of the dynamics in that system, but that intra-specific density-dependence, positive in hare and negative in lynx, also contributed substantially. This is consistent with empirical and experimental studies that ruled out the influence of adverse interactions with conspecifics on hare population growth, partly in line with low food constraints (Stenseth et al. 2002; Krebs et al. 2006). Negative density-dependence was also found in boreal lynx populations, as individuals tend to be more territorial before the population peak (Slough and Mowat 1996). What is more surprising is the positive intra-specific density-dependence in the hare, which contrasts with the absence of density-dependence found in other studies (Krebs et al. 2006). This result suggests that the hare population grows faster at high density. This could correspond to a number of biological scenarios, for instance, predation avoidance, or mating success, might increase at high density. Alternatively, this results can also be explained by an artifact in the sampling process of the data, which consists of pelt counts. It may be that a higher pelt count in the previous year has driven more trappers to go out and collect pelts the

following year, leading to an artificial increase in the hare population during periods of high hare density (Odum and Barrett 1972). Overall, our results hence demonstrate that NODEs can provide sensible biological insights in light of the socio-environmental dynamics of the system.

4.2 Comparison with related approaches

Traditionally, ecological dynamical systems such as the hare-lynx system are analysed with parameteric dynamical models, such as ODE models in continuous time (e.g. Deng 2018), and autoregressive models (or difference equation) in discrete time (e.g. Stenseth et al. 2002), which rely on specific mathematical constructions. The NODE approach provides non-parametric evidence for intra- and inter-specific effects in this system, which are thereby robust to assumptions about the nature of the ecological interaction between the hare and lynx population. More generally, parametric models require (i) a strong knowledge to formulate assumptions regarding the dynamical processes, (ii) advanced mathematical skills to translate these assumptions into parametric equations, and (iii) a considerable amount of model selection to find a suitable model, which becomes impractical with increasing process complexity. NODEs address each of these points, as ANNs (i) require a limited amount of assumptions, which merely consists in the specification of inputs, (ii) emulate infinitely many different process shapes, (iii) browse through them continuously, regardless of the complexity of the process. The main benefit of NODEs is hence that they permit the user to infer dynamical processes where complexity and lack of prior knowledge makes a classical parametric approach impractical, and otherwise provides first-hand information to guide the design and selection of parametric equations. In particular, NODEs provide a powerful alternative

to parametric models when it comes to the identification and categorisation of equilibrium points and steady-state behaviours empirically informed by time series.

In the context of the NODE literature, our study provides a first successful assessment of the suitability of NODEs to analyse real ecological time series and derive meaningful biological insights. We acknowledge that NODE models have been applied successfully in the past to model prey-predator dynamics, especially in the field of artificial intelligence (e.g. Mai, Shattuck, and O'Hern 2016; Rackauckas et al. 2019; Massaroli et al. 2020). This work was instrumental in establishing the workings and validity of the approach, and we also provide one such proof of validity in the supplementary material of the present work by analysing a simulated time series with known parameters and find an agreement between the true functions and the functions learned by the networks. However, none of the studies above considered real biological systems, and proposed steps to extract biological quantities from those, so that much work remains to be done to find real world applications for NODEs. We view our study as a step in this direction as we consider an iconic ecological real time series, and provide steps to derive biologically sensitive quantities such as ecological interactions, dynamical coupling, and equilibrium points. We further argue that the range of applications of NODEs exceeds largely those considered in this manuscript.

We view NODEs as beneficial when compared to pure non-parametric dynamical system approaches, such as recurrent neural networks (RNNs, e.g. Chon et al. 2001; Obach et al. 2001; Matsunaga, Rakocevic, and Brancher 2013), which rely on single ANNs to approximate the dynamics of the entire system. In doing so, RNNs are often criticised for their black box nature which

greatly reduces interpretability of the model, and its applicability as an explanatory tool, making them more suitable for forecasting. NODEs circumvent this problem by embedding ANNs in a consistent theoretical framework outlined by the parametric ODE equations, making ANNs more interpretable and meaningful, which is an idea that preceded the birth of NODEs (Aarts and Van Der Veer 2001). For instance, if we can assume that the life cycle of a given species is well known, we can model it in the NODE with specific life stage variables, use parametric functions for known transitions, and neural networks to learn unknown transition functions. By doing so, we progressively dissect ANNs into possible mechanisms, thus opening the black box (Aarts and Van Der Veer 2001).

We view that our work also improves over closely related non-parametric dynamical methods in ecology, such as semi-specified models (Wood 2001), gradient matching (Ellner, Seifu, and Smith 2002), and residual minimisation training (Wu, Fukuhara, and Takeda 2005). These studies have in common the idea of embedding non-parametric functions, such as splines and neural networks, into dynamical systems. However the work remained limited to inferring specific functions (e.g. density-dependence in recruitment rates, Ellner, Seifu, and Smith 2002), and did not consider system level properties, such as ecological interactions networks or equilibrium points, as the aim of the inference. Furthermore, each study provided their own mathematical constructions and way of fitting these models, which hindered uptake of the methodology. Here we propose to rely on the recently discovered framework of NODEs to widen the scope considered by these pioneering studies, and cast these models in an integrated Bayesian framework.

4.3 Further applications to ecological and evolutionary dynamics

The NODE system in our case study can be used to identify the drivers of the demography of populations from time series (Fig. 5, 1A and 1B), and is readily applicable to a range of other ecological interactions, whether it is to quantify competitive interactions (Gamelon et al. 2019) or trophic interactions (Hiltunen et al. 2013). This can be achieved by modelling changes in population densities with differential equations (Fig. 5, 1C), and by approximating demographic processes, such as per-capita growth rates, birth or death rates, consumption rates, with ANNs (Fig. 5, 1D). Then by analysing the system we can establish networks of ecological interactions and their contribution to the dynamics of each species in the community. In doing so, NODEs also provide a bridge between empirical systems and theoretical ecological interactions frameworks, such as that of Press Perturbation (Montoya et al. 2009), or classic trophic ODE models (Hiltunen et al. 2013).

Similarly, NODEs can be applied to identify the drivers of evolution in natural systems (Fig. 5, 2A) from time series of the traits, demography, and environmental variables (Fig. 5, 2B), such as those available for the Darwin's Finches system (Grant and Grant 1993). This can be done by defining a set of differential equations describing changes in phenotypic, demographic, and environmental states (Fig. 5, 2C), for instance by merging demographic models with the Price equation (Ellner, Geber, and Hairston 2011; Lion 2018), and by approximating the fitness landscape and fitness gradient with ANNs (Fig. 5, 2D). Following an application of the Geber method to both the fitness landscape and fitness gradient, we could derive the contribution of ecology and evolution to the dynamics of the phenotype and populations (Hairston et al. 2005). In this way NODEs provide an

511 ”equation free” (i.e. non-parametric) way of applying the Geber method, and of testing theoretical
512 frameworks for eco-evolutionary feedbacks in real time series, which would benefit many existing
513 studies in this area (e.g. Hairston et al. 2005; Van Velzen and Gaedke 2017; Pigeon et al. 2017;
514 Patel, Cortez, and Schreiber 2018; Lion 2018).

515 NODEs can also be used to learn the drivers of spatial dynamics of individuals and populations
516 (Fig. 5, 3A) from records of paths and trajectories (e.g. foraging, dispersal, migrations) (Fig.
517 5, 3B). This can be achieved by modelling the changes in the spatial position of individuals, or
518 populations with differential equations (Fig. 5, 3C), and approximate the movement kernels, that is
519 the probability of a given move depending on a set of cues, with ANNs (Fig. 5, 3D). We view this
520 last application of NODEs as particularly useful given that we often lack a consistent mathematical
521 framework to explain animal movement (Dalziel, Morales, and Fryxell 2008), and would lead to
522 novel insights if combined with theoretical frameworks for shoaling and flocking behaviours, or
523 flying predators (e.g. Olberg 2012; Corcoran and Conner 2016; Brighton et al. 2017).

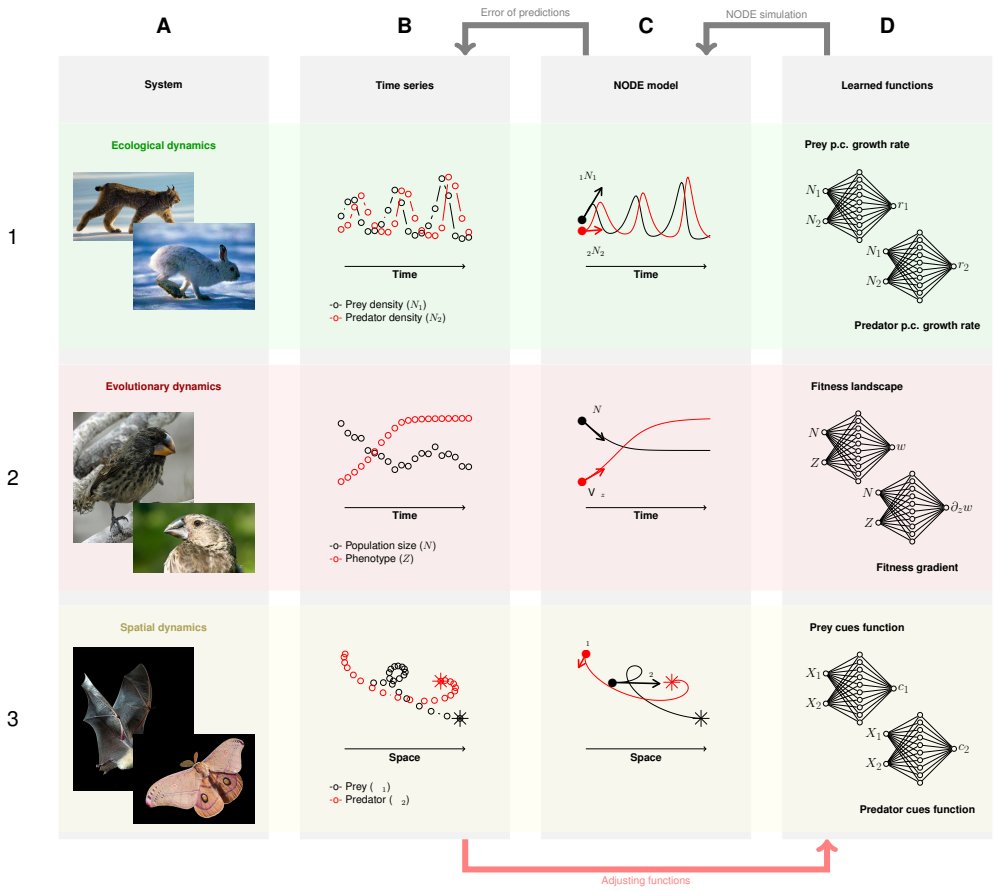

Figure 5: Possible applications of NODEs to ecological, evolutionary, and spatial dynamics. NODEs can be used to model a wide range of biological functions and systems, including (1) population dynamics, to learn ecological interaction networks beyond the hare-lynx system considered here, (2) evolutionary dynamics, where they could be used to learn fitness landscapes and gradients from time series of phenotypic change and population density, for example, and (3) in a spatial dynamics context, where they can be used to learn individual cues functions by analysing continuous time spatial trajectories, such as those of flying predators like bats, birds of prey, dragonflies.

4.4 Limits

The main limitation of the NODE approach is that they are hard to fit, due to a high number of network parameters and hence high computational costs. NODE and ODE systems in general need to be simulated for each set of parameters in order to compute the error with respect to the observations, contrary to linear models, or ANNs, which can be evaluated at all points in the time series simultaneously. Simulating the model through an ODE solver prevents the computation of gradients of the error with respect to each model parameter, which further prevents the use of standard gradient descent methods. That, in addition to the high number of network parameters, overall makes the training of these models challenging and computationally intensive (Chen et al. 2019). There have been steps taken to solve this issue, for instance by relying on highly sophisticated techniques such at automatic differentiation (Chen et al. 2019), and the adjoint sensitivity method (Rackauckas et al. 2019), but it is our view that the training of these models remains nonetheless intensive.

Conclusion

NODEs combine the explanatory power of dynamical mathematical models and the learning capacity of ANNs, giving them the potential to approximate the dynamics of any biological system based on simple time series data. This framework has not been applied yet, its potential to further our understanding of system dynamics anywhere theory is missing, is unexplored. We show that NODEs can be applied successfully to analyse time series in ecology, using the hare-lynx prey-predator system as a case-study. We further provided several directions for addressing key

questions in ecological, spatial, and evolutionary dynamics, with NODEs, highlighting its generalisability and its potential to generate new insights in ecology and evolution. Successfully applying and developing this framework will also result in concrete applications, as NODE systems could be used to control biological systems in real time, whether it is to maintain them at a maximum sustainable yield (e.g. in fisheries, agro-ecological systems), or to restore and protect them more efficiently against perturbations (e.g. invasive species, climate change).

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Statement of authorship

Willem Bonnaffé designed the method, performed the analysis, wrote the manuscript; Ben C. Sheldon provided input for the manuscript, commented on the manuscript; Tim Coulson led investigations, provided input for the manuscript, commented on the manuscript.

Data accessibility

All data and code is fully available at https://github.com/WillemBonnaffe/NODEs/tree/master/NODER and on Zenodo at https://doi.org/10.5281/zenodo.4630706 (Bonnaffe, Sheldon, and Coulson 2021).

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Part III

Chapter 3: On the repeatability of ecological interactions and dynamics in artificial replicated microcosms

On the repeatibility of ecological interactions and dynamics in an artificial replicated microcosm

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Specifications: 140 words in abstract; 7071 words in text; 40 references; 5 figures; 1 table

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Statement of authorship: Willem Bonnaffé designed the method, performed the analysis, wrote the manuscript; Tim Coulson led investigations, provided input for the manuscript, commented on the manuscript.

Abstract

Generalisation of dynamical processes across natural systems is difficult because they are complex and hard to observe. The hope is that generalisation may be achieved by adequately modelling the complexity of systems, and observe them in sufficient detail. We investigate this by looking at the consistency of ecological interactions across three replicates of a three-species prey-predator system, well-observed in an artificial environment, using neural ordinary differential equations. We find that dominant interactions are consistent across the replicates, while weaker interactions are not, leading to different dynamical patterns across replicated systems. Our study hence suggests that generalisation of dynamical processes across systems may not be possible, even in simpler systems in ideal monitoring conditions. This is a problem because if we are not able to make generalisations in a simple artificial system, how can we make generalisation in the real world?

1 Introduction

The repeatability of ecological and evolutionary dynamics varies widely across systems and species. Sticklebacks from different lakes in Canada have independently evolved to a similar river morph phenotype (Thompson, Taylor, and Mcphail 1997). In guppies, four replicated populations located in different streams in Trinidad evolved the same low-predation phenotype (Reznick, Bryga, and Endler 1990). Multiple studies in experimental microcosms, particularly in rotifer populations, have shown that population dynamics were broadly repeatable (Yoshida et al. 2003; Yoshida et al. 2007; Becks et al. 2010; Becks et al. 2012; Hiltunen et al. 2013). Overall, this demonstrated that ecological and evolutionary dynamics may be repeatable across different instances of the same system, at least qualitatively. This was a fascinating finding given the complexity of the mechanisms involved and the subtle variations in environmental conditions across the different populations.

These systems hinted at the possibility for identifying global, generalisable, dynamical models. In practice, however, generalising dynamics and dynamical processes (i.e. functional representations describing which and how state variables affect each other and determine system dynamics) across natural systems has proven difficult (Lawton 1999). First, even if the dynamical patterns, and their outcomes, may appear to be conserved across similar systems, they may be underpinned by different processes. For instance, the evolution of the sticklebacks to highly similar river-adapted phenotypes has been shown to be underpinned by radically different genetic alterations (Raeymaekers et al. 2017). Second, it is often unclear whether quantitative differences across replicated systems

arise from pure stochasticity (Dallas et al. 2021), observation error (De Meester et al. 2019), or deterministic changes in the dynamical processes. Finally, the complexity of biological processes themselves (Adamson and Morozov 2013), differences in genetic and environmental contexts, may prevent the identification of a suitable dynamical model. For example, Becks and colleagues found that differences in the initial amount of genetic variation in otherwise identical rotifer populations led to subtle changes to the dynamics (Becks et al. 2010). Different access to seed supplies can modify the strength of the interaction between a plant and its herbivore, leading to either stable or oscillatory dynamics (Bonsall, Van Der Meijden, and Crawley 2003). Differences in temperature can alter the ecological interaction structure of entire ecosystems (Shurin et al. 2012; Bonnaffé et al. 2021). Because of this, vital rates are often found to be inconsistent in time (Gross, Ives, and Nordheim 2005; Adamson and Morozov 2013), and space (e.g. Gamelon et al. 2019). Overall, a growing body of evidence shows that generalisation of dynamical processes across similar natural systems often fails (Lawton 1999, e.g. Kendall et al. 2005; Demyanov, Wood, and Kedwards 2006; Ezard, Côté, and Pelletier 2009).

So how could repeatable dynamics arise across multiple instances of the same system? We would expect dynamics to be repeatable if the components of the system (e.g. species), as well as interactions between components, are conserved. For this, populations should have similar distributions for the traits that underpin these interactions, and should further share the same environmental conditions, across instances. While this is unreasonable to expect from a natural system, it may be achievable in an artificial setting. In such a setting, it is possible to understand the structure of

the system, to control the environment, and to reduce observation error. So if we fail to identify and generalise dynamical models in natural systems, perhaps we may be able to do so in artificial systems.

In spite of this there are few studies that have attempted to characterise the generalisability of dynamics across replicated systems in a laboratory setting. In such a setting, idiosyncrasies in population dynamics can arise from (1) variations in ecological interactions and individual processes, as a result of evolution (e.g. Yoshida et al. 2003), or stochasticity (Dallas et al. 2021), (2) variations in initial conditions due to the experimental setting (Yoshida et al. 2003; Becks et al. 2010; De Meester et al. 2019), and (3) the complexity of the system which can lead to large changes in system dynamics with small changes in the system state and structure (Adamson and Morozov 2013). Two studies, one in aphids and the other in rotifers, found substantial variation in vital rates across replicated populations, by fitting a stage-structured population ODE model to population dynamics time series data (Bruijning, Jongejans, and Turcotte 2019; Rosenbaum et al. 2019). These studies hint that generalisability of population dynamical processes may not be possible because of intrinsic population structure and evolution, even in virtually identical populations hosted in artifical environments.

We identified three gaps in the literature. First, this kind of evidence remains scarce, due in part to the fact that dynamical modelling approaches guided by empirical data are still not widespread (Pontarp, Brännström, and Petchey 2019). Second, most of these studies relied on parametric frameworks, which impose arbitrary pre-determined forms for the dynamical processes at play, so

that their model may not capture properly the complexity of the dynamics of these populations (Jost and Ellner 2000; Adamson and Morozov 2013; Bonnaffé, Sheldon, and Coulson 2021). Finally, most studies usually analyse dynamics in single-species systems, but not multi-species systems, such as those with intraguild predation, which are more biologically realistic scenarios (Hiltunen et al. 2013). Further studies are consequently required to investigate the consistency of dynamical processes in simple multi-species and well-observed systems, to conclude about the generalisability of population dynamics across systems.

Our aim in this study is to provide an assessment of the repeatability of dynamical processes across different instances of a realistic multi-species system hosted in a well-observed environment. We do this by quantifying the direction, strength, and consistency of interactions in time and across replicates of a three-species microcosm in an experimental setting. We hypothesise that if the system is (1) simple enough, (2) well-observed, (3) in a controlled environment, then dynamical effects/interactions should be broadly consistent in time and across replicates, hence allowing for generalisation of dynamics across systems. We consider three replicates of a three-species system, consisting in a prey (algae), intermediate-predator (flagellate), and top-predator (rotifer). The algae is consumed by the flagellate and rotifer, and the flagellate is consumed by the rotifer. We use three replicated system runs from a study by Hiltunen and colleagues which feature sequential oscillations of the density of the three species (Hiltunen et al. 2013). We analyse the time series with neural ordinary differential equations (Bonnaffé, Sheldon, and Coulson 2021), which allows us to approximate non-parametrically population growth rates, and quantify the direction, strength,

and consistency of inter- and intra-specific effects on the growth of each population. We find that the interaction between the rotifer and algae is consistent throughout time and across replicates, while the interaction between the flagellate and the two other species is not. Our study suggests that dynamical processes may sometimes not be consistent and generalisable across systems, even when they are as close to identical as experimentation permits. We discuss these results and hint at the underlying impact of evolution driving differences in these systems.

2 Material and Methods

2.1 Method overview

The aim of the study is to determine the extent to which the strength and direction of interactions between three species in a tri-trophic prey-predator system are consistent in time and across replicates, as a way to assess the generalisibility of dynamics across simple and well-observed systems. To do this we approximate the dynamics of each species by fitting neural ordinary differential equations (NODEs, Bonnaffé, Sheldon, and Coulson 2021) to replicated time series data of changes in prey and predator densities. We then derive the interactions between species by looking at the sensitivity of the dynamics to a change in the density of each species, and assess their consistency in time and across replicates.

2.2 System

We consider a three-species laboratory microcosm consisting of an algal prey (*Chlorella autrophica*), a flagellate intermediate predator (*Oxyrrhis marina*), and a rotifer top predator (*Brachionus plicatilis*). The algal prey is consumed by the intermediate and top predator, the top predator also consumes the intermediate predator (Arndt 1993). The dynamics of this system, here the daily change in the density of each species, were recorded in three replicated time series experiments performed by Hiltunen and colleagues (Hiltunen et al. 2013, Fig. 1). The aim of their experiment was to determine which type of population dynamics would arise in a system with two predators competing for the same resource (the algae), where one predator (the rotifer) would also be able to consume its competitor (the flagellate). According to their expectations, they found prey-predator oscillations, where the lag between the density peaks of each species reflected their position in the food web. Namely that the peak of algae preceded the flagellate peak, which itself preceded the rotifer peak.

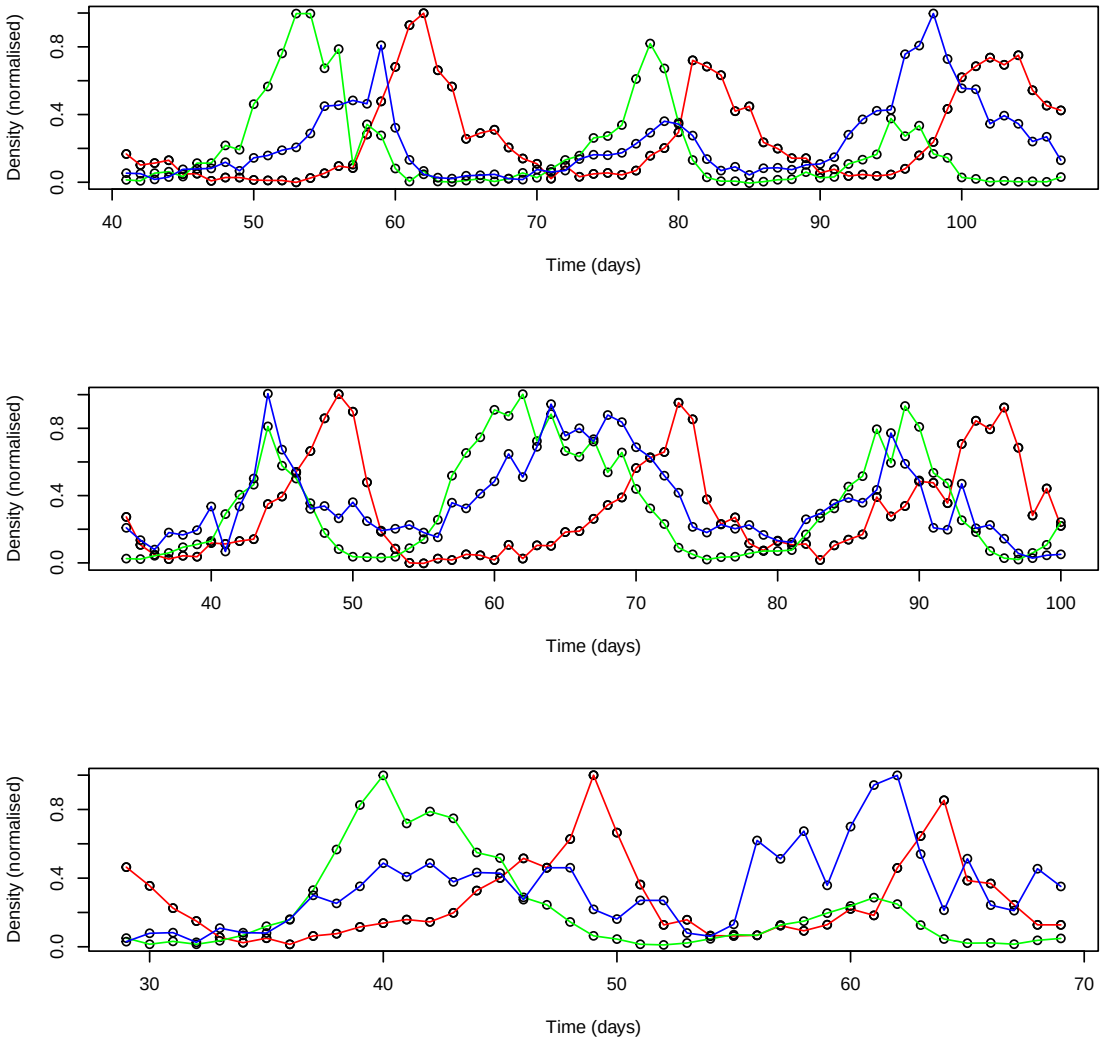

Figure 1: Time series of the prey algae (green), flagellate intermediate predator (blue), and top predator (red). Each time series corresponds to one of the three replicates. Black open dots correspond to observed densities, scaled between 0 and 1. Time series were obtained from the study by Hiltunen and colleagues (Hiltunen et al. 2013).

Their microcosms are close to true replicates in that environmental conditions, namely temperature, salinity, and nutrient influx, where maintained constant, and initial conditions, that is the initial density of each species, were shared across all replicates. In spite of that, they still found evidence for algae evolution in some parts of the time series, which resulted in a shift of the dynamics from fast prey-predator cycles to slower oscillations, similar to those documented in previous studies on similar systems (Yoshida et al. 2003; Becks et al. 2010), even in lineages where genetic variation in predator defense traits was eliminated at the start of the experiment. Consequently, the time series that they reported are the ones that did not present evidence of evolution, and therefore displayed purely ecological dynamics.

We use their time series because they describe a simple yet biologically realistic ecosystem, and because the quality of the replication of their microcosm reduces as much as possible observational and experimental error, and rules out environmental variation (Hiltunen et al. 2013). We digitised these time series by extracting by hand the coordinates of every points in the referential of the axis of the graph of the original study, and analysed them.

2.3 Model specifications

The aim of the modelling approach is to infer the drivers of the dynamics of each species from the time series data. More specifically, we want to quantify the effect of a change in the density of one species on the dynamics of the other species. In this way we can understand which, and to what extent, species interactions drive population dynamics. To do this we use neural ordi-

nary differential equation (NODEs), which is a novel methodology allowing us to infer dynamical processes non-parametrically from time series data (Bonnaffé, Sheldon, and Coulson 2021). We choose this methodology over traditional approaches because it offers two advantages. The first lies in the fact that NODEs approximate the dynamics of populations non-parametrically, and are therefore not subject to incorrect model specifications (Jost and Ellner 2000; Adamson and Morozov 2013). This is important as it offers an objective estimation of the inter-dependences between state variables, and hence a reliable assessment of whether a species is contributing to the dynamics of another. The second advantage is that it is a dynamical systems approach, which means that the effects are estimated in a dynamically consistent system of ODEs (Bonnaffé, Sheldon, and Coulson 2021). This is useful because it accounts for the dynamical nature of the system, so that it includes lag effects, not just direct correlations between variables.

We define a simple NODE system for the three-species system described previously

$$\begin{aligned} \frac{dR}{dt} &= r_R(R,G,B,\beta_R)R \\ \frac{dG}{dt} &= r_G(R,G,B,\beta_G)G \\ \frac{dB}{dt} &= r_B(R,G,B,\beta_B)B \end{aligned} \tag{1}$$

where dR/dt, dG/dt, and dB/dt denote the change in rotifer (R), algae (G), and flagellate (B) density in continuous time. The per-capita growth rates r_R, r_G, and r_B are non-parametric functions of the density R, G, B of each species. The shapes of the non-parametric functions are controlled by the parameter vectors β_R, β_G, and β_B. Fitting the NODE system (1) amounts to finding the

parameter vectors, and thereby the per-capita growth rates, that best describe the changes in density observed in the time series data.

Each non-parametric functions is an artificial neural network (ANN). ANNs are powerful mathematical objects that can be trained to approximate the shape of dynamical processes (Funahashi and Nakamura 1993; Chen and Chen 1993). For the sake of simplicity, we consider the simplest form of an ANN which contains a single hidden layer, namely a single layer peceptron (SLP)

$$r_R = \sum_{i=1}^{N} \beta_i f_\sigma \left(\beta_{i0} + \beta_{i1} R + \beta_{i2} G + \beta_{i3} B\right) \tag{2}$$

which takes as input the density of each species R, G, and B, and output the corresponding per-capita growth rate. The parameter vector β_R, β_G, β_B, contain the weight of the connections in the ANNs. The SLP can be viewed as a weighted sum of basis functions f_σ of the state variables of the system. In this study we consider sigmoid basis functions, as they are commonly used and their capacity to approximate any continuous function is well established theoretically (Funahashi and Nakamura 1993). The number of units in the hidden layer N is chosen to be 10, as this is a commonly used number for systems of that size (e.g. Wu, Fukuhara, and Takeda 2005). More details regarding these models can be found in our previous work (Bonnaffé, Sheldon, and Coulson 2021).

2.4 Model fitting

This section describes how to recover the parameters β of the NODE system given the time series data at hand. In a previous study, we developed an approach to fit NODE systems to time series data (Bonnaffé, Sheldon, and Coulson 2021). The technique relied on simulating the NODE system over the times covered by the time series, and then computing the difference between the predictions of the NODE model and the observations of the time series. The model is fitted to the time series by adjusting the parameter vectors until temporal dynamics of the state variables matched the observations as closely as possible. There are two caveats with this approach that we solve in this study by opting for a different fitting approach. The first caveat is that the fitting process previously described is computationally expensive, because the NODE system has to be simulated over the entire range of the data at every step of the optimisation. Second, the simulation prevents the computation of gradients of the posterior distribution of the model, and thereby prevents the use of efficient gradient descent approaches. Overall, this makes it hard to avoid getting trapped in local maxima.

Instead, we propose an alternative fitting approach, building on the work of Wu et al., and Ellner and colleagues, which relies on data interpolation to approximate populations state and dynamics (Ellner, Seifu, and Smith 2002; Wu, Fukuhara, and Takeda 2005). We proceed in two steps, (1) we interpolate the time series data to estimate the states and dynamics of each variable, and (2) we fit the NODE system directly to these estimated dynamics. In this way we avoid the simulation step as the NODE system can then be directly compared to the interpolated dynamics.

Interpolating the data

We interpolate the time series and differentiate it with respect to time in order to approximate the dynamics of the system. The interpolation is found via a non-parametric regression of the interpolating function on the time series data

$$Y(t_i) = \tilde{Y}(t_i, \Omega) + \varepsilon_i \tag{3}$$

where $Y(t_i)$ is the observed value of the variable at time t_i and $\tilde{Y}(t_i, \Omega)$ is the value predicted by the interpolating function, up to an error $\varepsilon_i \sim \mathcal{N}(0, \sigma_1)$. In the present case, the variables are either the rotifer density R, algae density G, or flagellate density B, depending on which time series is interpolated. The interpolating function is chosen to be an SLP with sinusoid activation functions

$$\tilde{Y}(t, \Omega) = \sum_{i=1}^{N} \omega_{i0} sin\left(\pi(\omega_{i1} + \omega_{i2} t)\right) \tag{4}$$

where $\tilde{Y}(t, \Omega)$ is the interpolated state variable, either R, G, or B, and is determined to be a weighted sum of sinusoid functions of time. The interpolation parameter vector Ω contains the weights ω_{i0}, ω_{i1}, and ω_{i2} which control the amplitude, shift, and frequency of the oscillations in the time series, respectively. We found sinusoid activation functions to be most efficient for interpolating population dynamics compared to other functions (such as sigmoid, hyperbolic). Following this approach

we obtain directly an approximation of the dynamics of the state variable by differentiating the SLP with respect to time

$$\frac{\partial}{\partial t}\tilde{Y}(t) = \sum_{i=1}^{N} \omega_{i0}\pi\omega_{i2}cos\left(\pi(\omega_{i1} + \omega_{i2}t)\right) \tag{5}$$

as well as an analytical expression of the interpolated per-capita growth rate of the populations, by combining equation (4) and (5)

$$\tilde{r}_Y = \frac{1}{\tilde{Y}}\frac{\partial \tilde{Y}}{\partial t} \tag{6}$$

Overall, interpolating the data amounts to finding the parameter vector Ω that minimises the error in equation (3). In practice, we log-transform the densities, to cast the variables on the real number space. This also allows us to re-write equation (6) in a more compact form, namely $\tilde{r}_Y = \frac{\partial}{\partial t}\log\tilde{Y}$. We standardise the log-densities with respect the their mean and standard deviation (i.e. $Z = (log(Y) - \mu)/\sigma$). This is to facilitate the training of the NODE by bringing the parameters in the neural network on the same scale.

Fitting NODEs to the interpolated data

The second step is to match the NODE system to the interpolated dynamics, given the interpolated state variables. Thanks to the interpolation of the data, this simply amounts to performing a regression of the non-parametric approximation of the per-capita growth rate (equation 2) on the

interpolated per-capita growth rate (equation 6)

$$\tilde{r}_Y(t_i) = r_Y(t_i, \beta) + \eta_i \tag{7}$$

up to an error term $\eta_i \sim \mathcal{N}(0, \sigma_2)$. For instance, the per-capita growth rate of the rotifer writes as $\tilde{r}_R(t_i) = r_R\left(\tilde{R}(t_i), \tilde{G}(t_i), \tilde{B}(t_i), \beta_R\right) + \eta_i$. Fitting the NODE per-capita growth rate hence amounts to finding the parameter vector β that minimises the error in equation 7, given the interpolation.

Statistical modelling approach

The following section describes how to recover the parameters for the interpolation and NODE system that best describe the time series, while controlling for overfitting. The fitting of the models is performed in a Bayesian framework, considering normal error structure for the residuals, and normal prior density distributions on the parameters

$$p(\theta|\mathscr{D}) \propto p(\mathscr{D}|\theta)p(\theta) \tag{8}$$

where θ is the parameter vector of the model, and $\mathscr{D}$ the evidence, namely the data that the model is fitted to. In the case of the interpolation, the evidence is the population densities, either $R(t)$, $G(t)$, or $B(t)$, and the parameters are the weights Ω in the sinusoid SLPs. In the case of fitting the NODE model to the interpolated data, the evidence is the interpolated per-capita growth rate of each population, either $\tilde{r}_R$, $\tilde{r}_G$, or $\tilde{r}_B$, and the parameters are the weights β_R, β_G, and β_B in the

non-parametric per-capita growth rates r_R, r_G, and r_B.

Assuming a normal likelihood for the residuals given the evidence we get

$$p(\mathscr{D}|\theta) = \prod_{i=1}^{I} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{e_i(\mathscr{D},\theta)^2}{2\sigma^2}\right\} \tag{9}$$

where $e_i(\mathscr{D},\theta)$ are the residuals of the model given the parameters. In the case of the interpolation, the residuals are $Y(t_i) - \tilde{Y}(t_i)$, and in the case of the NODE model, $\tilde{r}_Y(t_i) - r_Y(t_i)$. The dispersion term σ in the likelihood is measured by the parameters σ_1 in the case of the interpolation, and σ_2 in the case of the NODE fitting. I is the number of data points, either observations in the case of the interpolation, or interpolated points in the case of the NODE fitting.

The prior probability density functions for the parameters are given by

$$p(\theta) = \prod_{j=1}^{J} \frac{1}{\sqrt{2\pi\delta^2}} \exp\left\{-\frac{\theta_j^2}{2\delta^2}\right\} \tag{10}$$

where J is the number of parameters in the models. The parameter δ controls the dispersion of the priors, and thereby the complexity/level of constraint of the model.

There is no standard approach for choosing δ. Low values of dispersion may increase constraint on parameters too drastically, which would lead to underfitting, and result in a reduction of the variance of parameter estimates and bias mean estimates towards 0. In contrast, too high values of dispersion may lead to overfitting, by allowing for more complex shapes. To account for this, we

optimise the models on the second-level of inference. This means that we are finding the optimal value of δ, in addition to optimising the model parameters. We do this by optimising the marginal posterior density of the parameters, obtained by averaging out δ following a modification of the approach developped by Cawley and Talbot (Cawley and Talbot 2007). This yields the following expression for the marginal log posterior density of the parameters

$$\log P(\theta|\mathscr{D}) \propto \frac{I}{2}\log\left(1+\sum_{i=1}^{I} e_i(\mathscr{D},\theta)^2\right)+\frac{J}{2}\log\left(1+\sum_{j=1}^{J}\theta_j^2\right) \tag{11}$$

which amounts to optimising the log of the sum of squared residuals rather than the sum of squared residuals. $P(\theta|\mathscr{D})$ designates the marginal posterior distribution. More details on how to derive this expression from equation (8) can be found in a supplementary file (See supplementary A).

Finally, we estimate uncertainity in parameter values through anchor sampling, which produces approximate Bayesian estimates of the posterior distribution of the parameters (Pearce et al. 2018). The technique is simple in that it requires sampling a parameter vector from the prior distributions, and then optimising the posterior distribution from this starting point. By repeatedly taking samples, the sampled distribution approaches the posterior distribution and provides estimates and error around the quantities that can be derived from the models. The expectation of the quantities can then be approached by computing the mean of the approximated posterior distributions. The great strength of this approach is that it is unlikely to get stuck in local maxima and provides a more robust optimisation of the posterior. In this study, we took 100 posterior samples for each

time series, namely a hundred samples for the interpolation, and another hundred for the fitting of the NODE. The initial value of the parameters were picked from a random normal distribution with parameters $\sigma \geq 0.4$, which prevented underfitting the time series. We insured that there was moderate temporal autocorrelation and normality by visualising the residuals of the models. We also insured that the results were repeatable by running the entire fitting process a second time. We did not perform cross validation of results as we were only interested in estimating effects within the time series considered, rather than predicting future time steps.

2.5 Model analysis

We analyse the shape of the per-capita growth rates to recover the interaction between the three species in the system. In particular, we look at the effect and contribution of each species to the dynamics of the other. The effect is computed as the sensitivity (i.e. the gradient) of the per-capita growth rate of a given species with respect to the density of the other species. The contribution is computed following the Geber method (Hairston et al. 2005), which comes down to multiplying the dynamics of a variable by its effects on the other variables. We further compute the importance of a species in driving the dynamics of another by computing its relative contribution compared to other species at each time step. More details on how to recover these quantities can be found in our previous study (Bonnaffé, Sheldon, and Coulson 2021).

3 Results

We analyse sequentially the dynamics of each species, focussing on the amount of variation in per-capita growth rates explained by the NODE model, the overall direction, consistency, and importance of ecological interactions, and differences across replicates. Results are summarised in Table 1 and described in details for each species in the following section.

Table 1: Summary analysis. r^2 corresponds to the r squared of the NODE non-parametric approximation of the pre-capita growth rate compared to the interpolated per-capita growth rate for each of the three species. Mean effects are obtained by averaging the effect of one species on the growth rate of another throughout the time series. The % of total contributions is obtained by summing the square of contributions of one species density to the growth of the other at each time step throughout the time series, then by computing the proportion of total change that it accounts for.

			R	G	B
Replicate A	r^2		0.968	0.839	0.831
	Mean effects	on R	1.180	1.723	0.632
		on G	-1.888	-1.286	-0.208
		on B	-1.476	-0.371	0.131
	% of total contributions	to R	0.356	0.552	0.091
		to G	0.583	0.399	0.016
		to B	0.785	0.194	0.020
Replicate B	r^2		0.744	0.997	0.765
	Mean effects	on R	0.058	1.146	0.113
		on G	-1.505	0.707	-1.287
		on B	-1.000	0.505	-0.046
	% of total contributions	to R	0.035	0.934	0.029
		to G	0.439	0.242	0.317
		to B	0.624	0.373	0.001
Replicate C	r^2		0.923	0.962	0.726
	Mean effects	on R	-0.106	0.7814	0.498
		on G	-1.234	-0.1840	0.146
		on B	-0.659	0.0912	0.014
	% of total contributions	to R	0.080	0.743	0.175
		to G	0.900	0.068	0.030
		to B	0.913	0.084	0.001

Drivers of top predator dynamics

Figure 2 presents the drivers of the dynamics of rotifer. The NODE approximation of the per-capita growth rate fits quite well the interpolated per-capita growth rate across all replicates (Fig. 2, A2 B2 and C2, $r^2 > 0.7$, Table 1). The analysis of effects reveals overall a positive effect of algae on rotifer growth in all replicates (Fig. 2, A3, B3, C3, green line). The intermediate predator has a positive effect on rotifer growth in replicates A and C only (Fig. 2, A3, B3, C3, blue line). We find positive intra-specific density-dependence in the first replicate only (Fig. 2, A3, red line). Overall, all effects are consistent throughout the time series. The algae is the dominant driver of rotifer dynamics as it accounts for 55%, 93%, and 74% of the change in per-capita growth rates across the three replicates (Table 1, Fig. 2, A5, B5, C5, green line).

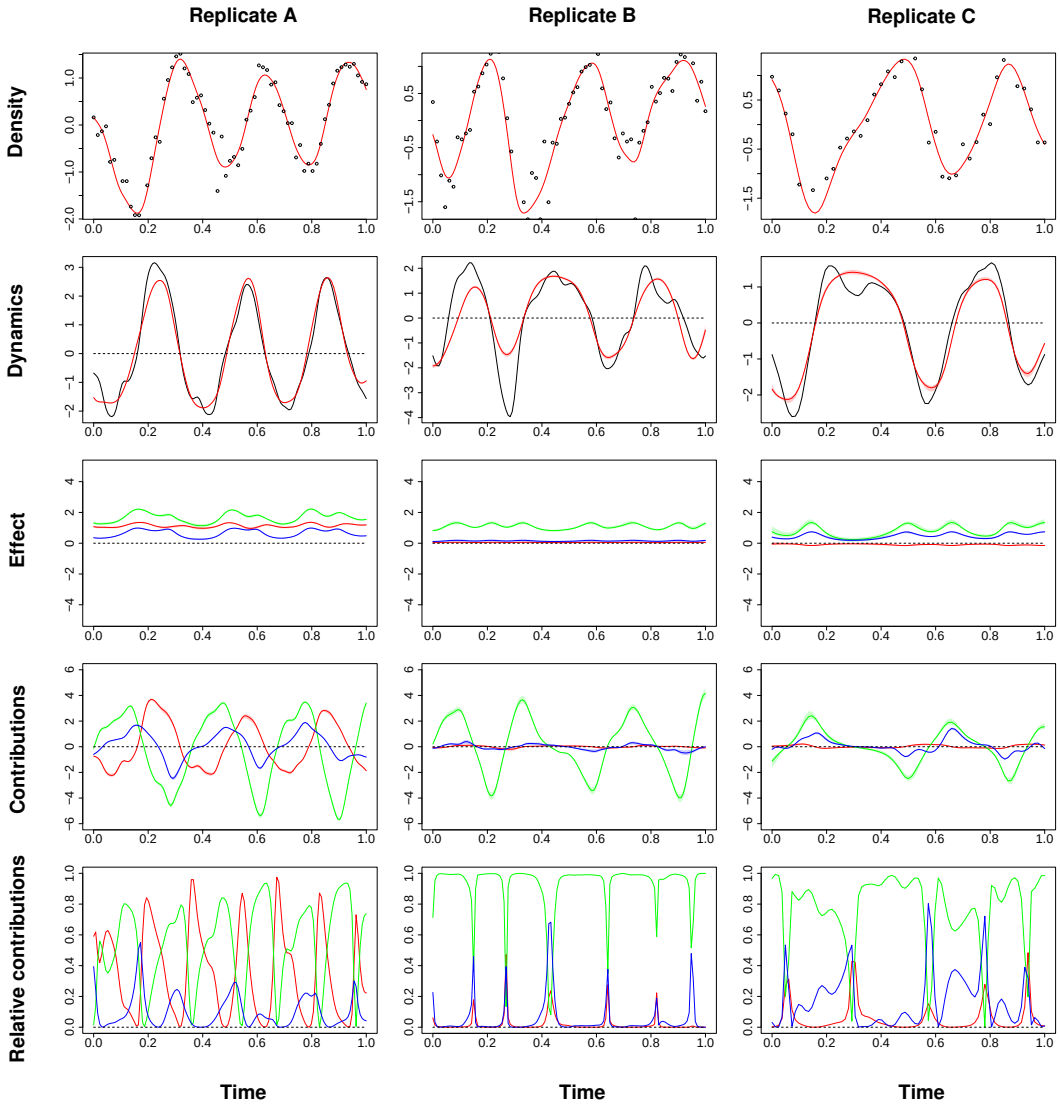

Figure 2: Drivers of rotifer dynamics. Row 1 presents the log density of rotifers in time, the dots are the observed densities while the red line is the interpolated data. Row 2 presents the change in log density at each time step, where the black line is the per-capita growth rate derived from the interpolated data and the red line is the NODE approximation. Row 3 presents the effect of each species on the dynamics/growth of rotifers, obtained by computing the sensitivity of the NODE approximation of the rotifer per-capita growth rate with respect to each species density. Row 4 presents the contribution of each species to the growth of the rotifer, obtained by multiplying its effect by its net change (i.e. row 2 and 3). Row 5 is the same as fourth but expressed as the proportion of total change at each time step explained by each species. For all figures, green, blue, and red refer respectively to algae, flagellate, and rotifer.

Drivers of the prey dynamics

The per-capita growth rate of the algae is well explained by the NODE approximation (Fig. 3, A2, B2, C2, $r^2 > 0.8$, Table 1). Overall, rotifers have a negative impact on the growth of algae in all replicates (Fig. 3, A3, B3, C3, red line). We find evidence for negative density-dependence in replicate A and positive density-dependence in replicate B, but not in replicate C (Fig. 3, A3, B3, C3, green line). The intermediate predator has an overall negative effect on Algae only in replicate B (Fig. 3, B3, blue line). The main driver of algae dynamics is the rotifer population, which accounts for 58%, 44%, and 90% of the change in algae per-capita growth rate across the three replicates. Density-dependence, however, plays a role in replicate A and B, with 40% and 24% of total change in growth, respectively (Table 1). The intermediate predator contributes only to algae growth in replicate B, accounting for 32% change in growth (Table 1). Overall, effects are found to be consistent throughout the time series except in replicate B (Fig. 3, B3), where effects vary in complicated ways, leading to a period in the time series where the algae is mostly driven by the intermediate predator and positive density-dependence, and less impacted by the top predator (Fig. 3, B5, from time 3 to 7.5).

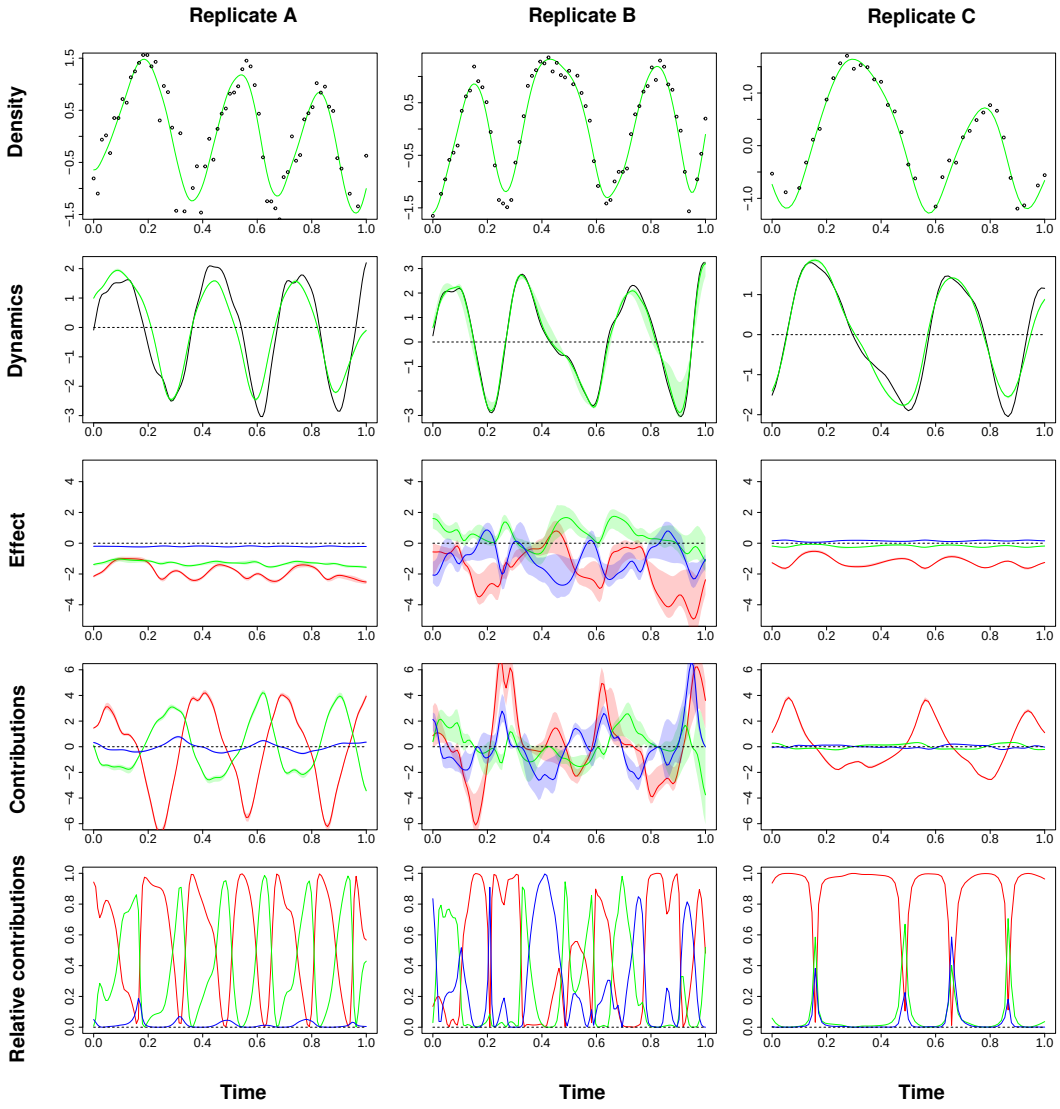

Figure 3: Drivers of algae dynamics. Row 1 presents the log density of algae in time, the dots are the observed densities while the green line is the interpolated data. Row 2 presents the change in log density at each time step, where the black line is the per-capita growth rate derived from the interpolated data and the green line is the NODE approximation. Row 3 presents the effect of each species on the dynamics/growth of algae, obtained by computing the sensitivity of the NODE approximation of the algae per-capita growth rate with respect to each species density. Row 4 presents the contribution of each species to the growth of the algae, obtained by multiplying its effect by its net change (i.e. row 2 and 3). Row 5 is the same as fourth but expressed as the proportion of total change at each time step explained by each species. For all figures, green, blue, and red refer respectively to algae, flagellate, and rotifer.

Drivers of the intermediate predator dynamics

The per-capita growth rate of the intermediate predator is quite well captured by the NODE approximation (Fig. 4, A2, B2, C2, $r^2 > 0.7$, Table 1). The intermediate predator is mainly negatively affected by the rotifer population (Fig. 4, A3, B3, C3, red line). The algae has a negative effect on flagellate growth in replicate A, and a positive one in replicate B (Fig. 4, A3, B3, green line). The rotifer predator dynamics accounts for 78%, 62%, 91% of the change in the flagellate growth rate, and the algae 20% and 37% in replicate A and B, respectively (Table 1, Fig. 4, A5, B5, C5). Overall, effects are consistent throughout the time series.

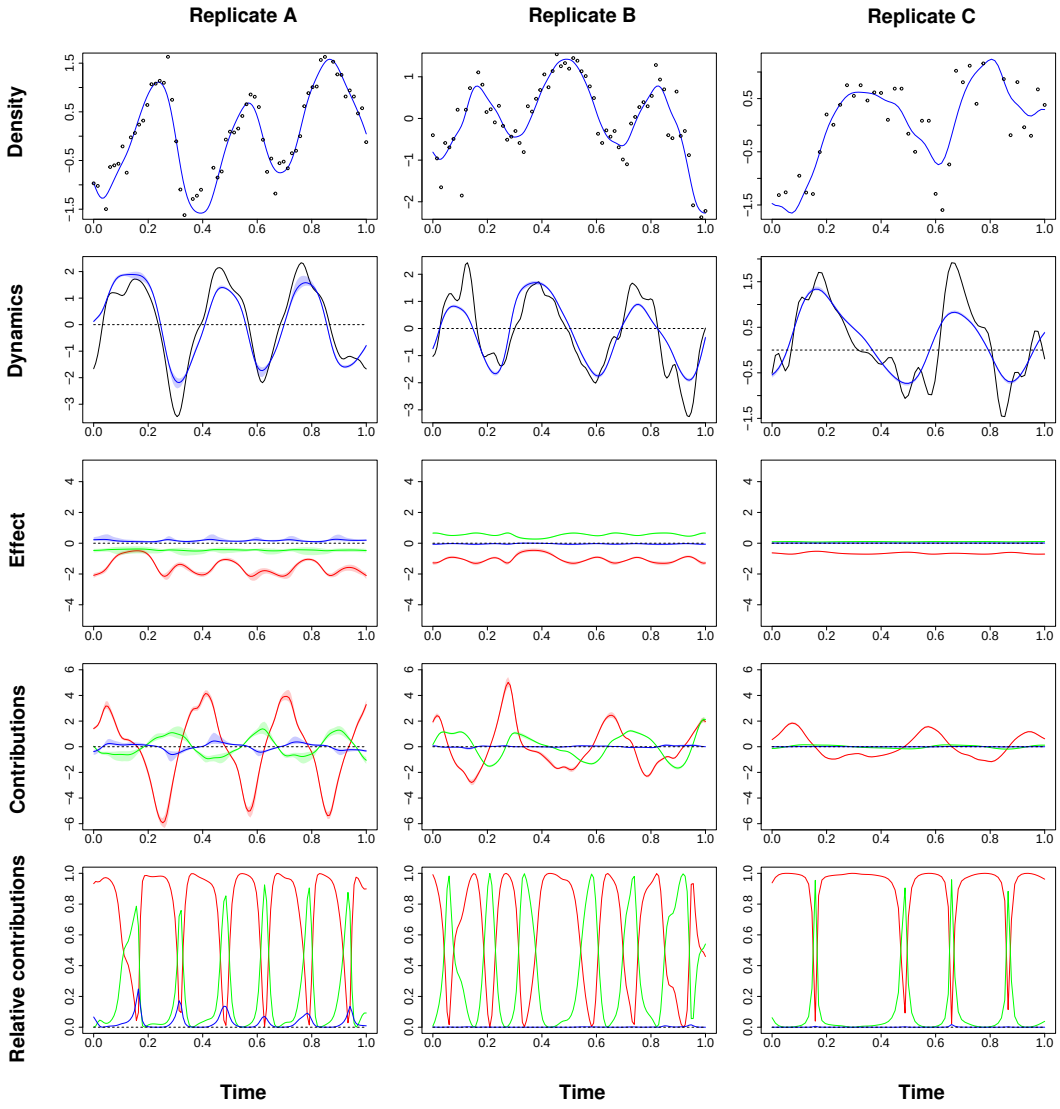

Figure 4: Drivers of flagellate dynamics. Row 1 presents the log density of flagellate in time, the dots are the observed densities while the blue line is the interpolated data. Row 2 presents the change in log density at each time step, where the black line is the per-capita growth rate derived from the interpolated data and the blue line is the NODE approximation. Row 3 presents the effect of each species on the dynamics/growth of flagellate, obtained by computing the sensitivity of the NODE approximation of the algae per-capita growth rate with respect to each species density. Row 4 presents the contribution of each species to the growth of the flagellate, obtained by multiplying its effect by its net change (i.e. row 2 and 3). Row 5 is the same as fourth but expressed as the proportion of total change at each time step explained by each species. For all figures, green, blue, and red refer respectively to algae, flagellate, and rotifer.

4 Discussion

Our ability to generalise dynamical processes and patterns across populations and communities is limited by the complexity of the processes, differences in environments, and incomplete and/or erroneous observations. It remains unclear to what extent generalisation would be possible if we overcame these limitations. We tackle this question by looking at the consistency of dynamical patterns across three replicated runs of a simple three-species community, hosted in identical environmental conditions in the lab. We expected to find consistency in the drivers of population dynamics, both in time and across replicates, and thereby demonstrate that generalisation of dynamical processes may be possible if the system states were well-observed and environmental conditions were known. To verify this expectation we (1) characterised the amount of variation in per-capita growth rates that is explainable deterministically, (2) quantified the direction, strength, and importance of ecological interactions for the growth of each population, and (3) described how these varied in time and across replicates. Our results are summarised in Figure 5. We find that only the effect of algae on rotifer ($G \to R$), and that of rotifer on algae ($R \to G$) and flagellate ($R \to B$) are conserved across the replicates. We find strong variation in the direction and importance of intra-specific density-dependence in rotifer ($R \to R$) and algae ($G \to G$) growth across the three replicates. The role played by the intermediate predator in the system was also different in all replicates, in that it only contributed substantially to the dynamics of the algae in replicate B ($B \to G$), and was either negatively, positively, or not affected by the algae ($G \to B$). Overall, this shows that the dominant interactions are conserved across replicates, but that minor interactions

328 vary substantially in importance and effect. Furthermore, we find that these dynamical processes
329 are more consistent in time within a system, than across replicates. Our results demonstrate that
330 because of partially generalisable dynamical processes, dynamical patterns may not be generalis-
331 able across systems, even with limited observation error and when environmental conditions and
332 community structure are conserved.

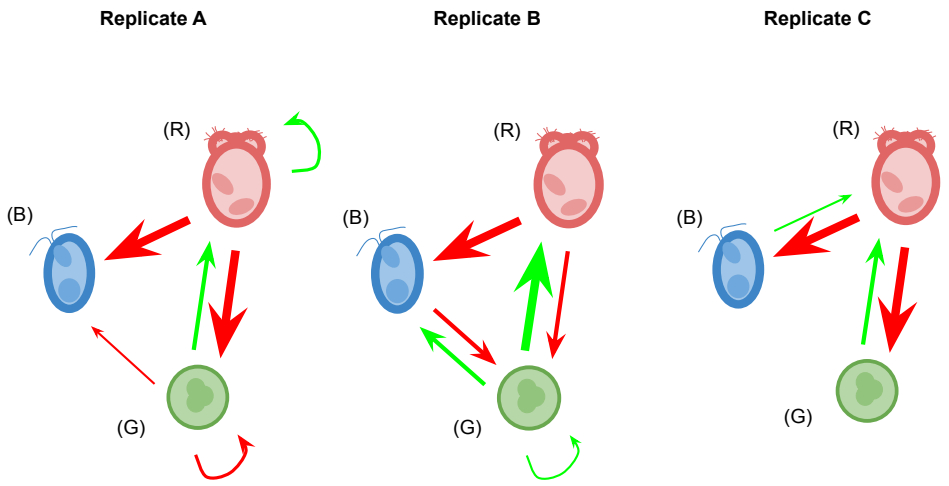

Figure 5: Interaction network inferred from the NODE analysis of the time series. The nodes G, R, B correspond to the algae, rotifer, and flagellate, respectively. Red and green arrows correspond to negative or positive mean effects, estimated by averaging the gradient of the per-capita growth rate of each species with respect to the density of the others across the time series. The width of the arrow is proportional to the % of total contributions of a variable on another, obtained by summing the square of contributions of one species density to the growth of the other at each time step throughout the time series, then by computing the proportion of total change that it accounts for.

Overall, our results are consistent with the biology of the system. The rotifer top-predator is found to have a strong negative impact on the two other species, in spite of variation in prey preference across replicates. This is consistent with previous study which have established the importance of rotifers for top-down control of flagellate and algal populations (Arndt 1993; Hiltunen et al. 2013). What is more suprising is the positive intra-specific density-dependence in the growth rate of the rotifer population in replicate A. This implies that the population of rotifer grows more at high density. This might be explained by various biological mechanisms, such as cannibalism (Gilbert 1976), though evidence remains limited in the *Brachionus* genus, or higher mating success at high density (Snell and Garman 1986). Similarly, the algae shows signs of positive intra-specific density-dependence in replicate B, though this effect remains confined to a brief period in the time series. This may be due to a higher chance of evading predators at high-density. This shows that the NODEs approach used here recovers results consistent with existing knowledge, but also identify subtle, more intriguing dynamical processes.

What might be the drivers of differences in the dynamical processes across these three replicates? One of the main source of variation in dynamics may be differences in the intrinsic structure of populations, such as variation in traits influencing intra- and inter-specific interactions which may lead to different dynamics (Yoshida et al. 2003; Yoshida et al. 2007; De Meester et al. 2019; Bruijning, Jongejans, and Turcotte 2019). Differences in the phenotypic structure may be due to unaccounted variation in initial conditions (Becks et al. 2010), or variation that developed throughout time as a result of evolution (e.g. Yoshida et al. 2003; Yoshida et al. 2007). In particular, the

algae in this system is prone to evolve a predator defence behaviour, by forming clumps, which reduce predation risk (Yoshida et al. 2003; Hiltunen et al. 2013). In their original paper, the authors limited the initial genetic diversity in the algae and focussed on replicates which did not display evidence of evolution, in an attempt to limit the impact of initial variation in phenotypic structure, and of evolution, on the dynamics (Hiltunen et al. 2013). In spite of that, evolution may not be eliminated completely, thus variation in traits governing the interactions between the species in the system may still have developed during the experiment, and led to changes in the dynamical processes across replicates. This would further be consistent with results from Yoshida and colleagues, who showed that evolution of prey defense could lead to ecological dynamics inconsistent with the known trophic interactions (Yoshida et al. 2007). Becks and colleagues also showed that small changes in the initial genotypic diversity could lead to drastically different eco-evolutionary dynamics (Becks et al. 2010). Our study hence reinforces the idea that rapid evolution may prevent generalisation of dynamical processes (Ezard, Côté, and Pelletier 2009; De Meester et al. 2019), and further suggests that this may also be the case in simple systems with limited environmental variation and opportunity for evolution.

Alternatively, stochasticity may be a major driver of differences across systems (Dallas et al. 2021). First, stochasticity in initial conditions, arising from the sampling of the communities of each replicate, could introduce differences in the interactions between the three populations. Second, stochasticity in the population dynamics themselves may result in different changes in densitiy levels in communities that are otherwise identical. Because our modelling approach is deterministic,

it does not directly provide an estimate of the total variation explained by stochasticity. Our modelling approach decomposes the variation in the data into observation and process error (Calder et al. 2003). First, the interpolation step introduces residual observation error, namely variation that is not captured by the interpolation. Second, the fitting of the NODE to the interpolation introduces residual process error, which is variation in the observation model that is not explained by the process modelled by the NODE. Stochasticity in the dynamics could explain the observation and process residual error (Calder et al. 2003), while stochasticity in initial conditions can only influence differences across replicates. Yet, we find relatively small process and observation error ($> 70\%$ of variance explained). So that, the dynamics of the three species are well explained by relatively simple linear deterministic effects between the state variables, which means that though dynamical processes differ across replicates they are reasonably consistent in time within each system. This suggests that stochasticity in dynamics plays a minor role in driving differences in dynamics across replicates, compared to stochasticity in initial conditions. In order to quantify this, we would need to estimate the influence of stochasticity directly. This can be done by modelling explicitly the random distribution of model parameters that underpin the dynamics of populations, which would then inform us about the importance of stochasticity driven by variation at the individual-level (Fox and Kendall 2002). Additionally, we could model stochasticity explicitly in the model with neural stochastic differential equations, which would allow us to separate the amount of change explainable by the deterministic part of the model, from demographic stochasticity, at each time step (Jia and Benson 2019).

393 Finally, we cannot exclude the potential contribution of unobserved variables that were not moni-
394 tored during the experiment, such as variation in nutrient levels in the chemostat, and which may
395 also lead to differences in the predation and intra-specific interactions across systems (e.g. Bonsall,
396 Van Der Meijden, and Crawley 2003; Fussmann and Blasius 2005; Posey, Alphin, and Cahoon
397 2006).

398 Should we expect limited generalisability of dynamics across systems, even if the complexity of
399 the process is properly captured, environmental conditions known, and the system well-observed?
400 A similar study, that inferred dynamical processes consistency from replicated time series of a
401 simple rotifer system, found substantial variation in vital rates across replicates (Rosenbaum et al.
402 2019), also pointing at a low generalisability of dynamical processes. Yet, the level of replication
403 of the time series of their studies was not as stringent as that of the time series we considered,
404 which leaves room for variability in dynamics to be caused by differences in experimental setup,
405 population history, initial densities. Bruijning and colleagues also found substantial variation in
406 vital rates across clones in a replicated system of aphids, showing that slight phenotypic variations
407 can change the population dynamics, all else being equal (Bruijning, Jongejans, and Turcotte 2019).
408 This phenomenon is likely to be even more important in more complicated systems and in a natural
409 setting where most variables are unobserved, which poses a problem for the generalisation of results
410 across studies and systems (De Meester et al. 2019). How can we expect to generalise dynamics
411 across real systems if we are not able to do so in artificial systems? Overall, our study reinforces
412 the view that general inferences should not be drawn from a single system, and that more efforts

are required to distinguish dynamical patterns that are conserved across systems from idiosyncratic ones.

Can we trust our models then if they are doomed to provide partly idiosyncratic answers? Our study demonstrates that processes can vary substantially across replicates, so that there may hence not be a single suitable functional form and parametrisation to model them (Lawton 1999). Yet, most of the work to date has involved fitting parametric models to time series data (e.g. Bruijning, Jongejans, and Turcotte 2019; Pontarp, Brännström, and Petchey 2019; Rosenbaum et al. 2019), which provide a very narrow view of the range of possible functions to describe the biological processes at play (Jost and Ellner 2000; Adamson and Morozov 2013). These models are subjective by nature (Jost and Ellner 2000; Adamson and Morozov 2013), and hence not generalisable, so that they greatly reduce our chance at identifying dynamical processes that are idiosyncratic, and those that are transferable.

What alternatives do we have then? We propose that NODEs are a suitable framework to study dynamical processes, as they produce inferences that are free of model assumption and facilitate comparison across studies and systems (Bonnaffé, Sheldon, and Coulson 2021). In this sense, our study already provides a potentially more objective depiction of dynamical processes than previous work with parametric models. Furthermore, in this paper we overcame the practical challenges of implementing NODEs by providing a computationally efficient fitting procedure, relying on time series interpolation, and developed a model selection criterion robust to overfitting. Similar approaches have been proposed in the past, for instance Ellner and colleagues developed a method

called gradient matching where they interpolated the data with cubic splines to which they fitted the differential equations (Jost and Ellner 2000; Ellner, Seifu, and Smith 2002). Wu and colleagues also relied on data interpolation of the data with ANNs to fit non-parametric approximations of population vital rates (Wu, Fukuhara, and Takeda 2005). But the approaches were too challenging and cumbersome to be implemented routinely, and were not used to tackle ecological interactions. Overall, our work demonstrates the usefulness of NODEs for inferring ecological interactions from count time series, which could readily be applied to a substantial pool of time series data.

Conclusion

Generalising dynamics across biological systems is hard because of the complexity of the dynamical processes (e.g. ecological interactions), differences in environmental context, and monitoring limitations. It remains unclear whether we could generalise dynamics if we properly modelled complexity, controlled for environmental effects, and observed systems precisely. We addressed this question by looking at the generalisability of dynamical processes across three replicated time series of a three-species system, using the novel framework of NODEs. We found that only the dominant interactions were conserved across the three time series, namely that between the algae and the rotifer, while the role of the intermediate predator varied substantially. Our results hence suggest that generalisation may not seem possible, even in simple system with no environmental variation. Given previous work in this system, the main cause of differences across replicates may be evolution in prey defence traits. We conclude that more work is required, using NODEs, to identify dynamical patterns that are conserved and those that are idiosyncratic across a wider range

of systems.

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Data accessibility

All data and code will be made fully available at https://github.com/WillemBonnaffe/NODER/rotifer.

Statement of authorship

Willem Bonnaffé designed the method, performed the analysis, wrote the manuscript; Tim Coulson led investigations, provided input for the manuscript, commented on the manuscript.

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5 Supplementary

A Bayesian regularisation

In this section we describe how to derive the modified model selection critieria developed by Cawley and Talbot (Cawley and Talbot 2007). Bayesian regularisation simply amounts to constraining the values of the parameters in the model to be close to a desired value. Usually, parameters are constrained by choosing normal priors centered about 0. In this case, the standard deviation of the normal priors governs the range of values that the parameters can take, and hence constrains more or less strongly the behaviour of the model (Cawley and Talbot 2007). Performing inference on the second level means that we are trying to find the appropriate value of the dispersion of the priors, in other words, the appropriate level of constraint on the model. In practice, choosing the level of constraint is difficult, Cawley and Talbot hence developed a criterion to perform model selection on the second level of inference. They proposed to optimise the marginal posterior distribution by averaging out the dispersion of the priors. With an appropriate choice of prior, the dispersion can be integrated out, leaving us with a formula for the posterior that only depends on the parameters of the model,

$$\log P(\theta|\mathscr{D}) \propto \frac{I}{2}\log\left(\sum_{i=1}^{I} e_i(\mathscr{D},\theta)^2\right) + \frac{J}{2}\log\left(\sum_{j=1}^{J}\theta_j^2\right) \tag{12}$$

where $P(\theta|\mathscr{D})$ denotes the marginal posterior density, $\mathscr{D}$ denotes the evidence, I and J denote the

number of data points and parameters, respectively, e_i denote the residuals of the model, and θ denote the parameters of the model. The construction is elegant because it is not sensitive to the choice of prior hyperparameters, and simple as it amounts to optimising the log of the sum of squares, rather than the sum of squares (in the case of normal ordinary least square).

The issue with this formula is that the marginal posterior density is infinity when the parameters are 0, which leads to underfitting. In this paper we use a modified criterion, which corrects for that problem

$$\log P(\theta|\mathscr{D}) \propto \frac{I}{2}\log\left(1+\sum_{i=1}^{I} e_i(\mathscr{D},\theta)^2\right)+\frac{J}{2}\log\left(1+\sum_{j=1}^{J}\theta_j^2\right) \tag{13}$$

where the marginal posterior density depends only on the residuals of the model when the parameters are equal to 0, and otherwise depends on both the parameters and the residudals. This construction can be obtained simply by assuming a gamma prior for the parameters $p(\xi) \propto \frac{1}{\xi}\exp\{-\xi\}$, where ξ is the regularisation parameter, instead of the improper Jeffreys' prior that Cawley and Talbot used in their original study, namely $p(\xi) \propto \frac{1}{\xi}$. The details of the integration of the posterior distribution over ξ can be found in Cawley and Talbot's orginal paper.

Part IV

Chapter 4: Comparison of eco-evolutionary feedback structure between *G. fortis* and *G. scandens* with neural ordinary differential equations

Comparison of eco-evolutionary feedback structure between *G. fortis* and *G. scandens* with neural ordinary differential equation

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Abstract

It is hard to identify eco-evolutionary feedback effects in natural systems. There are three main challenges that remain unaddressed: (1) comparing feedback structure between two closely related species in the same system, (2) assessing three-way feedbacks between resource-level, density, and phenotype, and (3) assessing the non-linearity of effects. We investigate these by inferring the drivers of ecological and evolutionary change in Darwin's finches. We use the novel framework of neural ordinary differential equations to quantify the effects of environmental, ecological, evolutionary variables on the dynamics of the system. We compare results across the two species present on the island *G. fortis* and *G. scandens*. Rainfall was a major driver of all dynamics in the system, but traits also contributed substantially to ecological dynamics. We find that feedbacks in *G. fortis* involved population dynamics and resource dynamics. In contrast, feedbacks in *G. scandens* were not coupled with demography, and mainly involved the resource. Our study hence shows that feedbacks differ between closely related species, and confirms the strong impact of phenotypic change in driving dynamics of entire ecosystems.

1 Introduction

There is evidence that evolution proceeds on ecological time scales, allowing for a coupling between evolutionnary and ecological change through so-called eco-evolutionary feedbacks (Pelletier, Garant, and Hendry 2009; Post and Palkovacs 2009; Schoener 2011). Eco-evolutionary feedbacks arise when evolutionary change in a given phenotype influences the demography of the population, and in turn the changes in the population state change the dynamics of the phenotype (Pelletier, Garant, and Hendry 2009). Eco-evolutionary feedbacks can also operate through changes in the environment of the organisms, for instance by changing the resource composition in the ecosystem, thereby altering selective pressures on the phenotype (Schoener 2011; Govaert et al. 2019).

The presence or absence of eco-evolutionary feedbacks have been shown to affect the dynamics of entire ecosystems (Bassar et al. 2015; Simon et al. 2017). For instance, experimental work showed that facilitating the evolution of predator defenses in a prey could result in eco-evolutionary cycles similar to prey-predator oscillations (Yoshida et al. 2003; Becks et al. 2010). In the wild, the rapid evolution of guppies from high predation phenotypes to low predation phenotype led to lower algal standing biomass and increased invetebrates biomass (e.g. Simon et al. 2017). In the Galapagos, the drastic change in seed composition on Daphne Major island that followed an exceptionally wet year triggered a rapid evolutionary change in beak morphology in two species of finches (e.g. Grant and Grant 1993). These iconic systems inspired a rapidly growing body of studies suggesting that eco-evolutionary feedbacks might be ubiquitous contributors to the dynamics of natural systems.

Yet, there are several elements about characterising fast evolutionary responses in natural systems that remain a challenge. First, pathways for feedbacks described in studies are often incomplete (Brunner et al. 2019). Most studies considered the evo-to-eco pathway, the reciprocal analysis, that considers the impact of population dynamics on evolutionary dynamics, is often lacking, which prevents us from quantifying the strength of the eco-evolutionary feedback (Benthem et al. 2017; Brunner et al. 2019; De Meester et al. 2019). Most studies focussed on simple feedback effects between population density and phenotypic change. Fewer studies considered feedbacks through indirect effects (Hendry 2019), such as changes in resource supplies, in spite of evidence suggesting that they may be important drivers of eco-evolutionary dynamics (e.g. Simon et al. 2017). In addition, most studies do not usually consider multiple species and traits within the same system, and hence provide an incomplete view the dynamical feedbacks (De Meester et al. 2019). It is hence still unknown whether and how multiple feedbacks in different species and traits may unfold simultaneously.

Second, there is currently a wealth of qualitative indirect evidence for eco-evolutionary feedbacks, but quantitative evidence regarding the importance of these effects for the dynamics of the system is often lacking, especially compared to environmental effects (Benthem et al. 2017; Hendry 2019). The few empirical studies that estimated effects of phenotypic change on ecological dynamics, and vice versa, found contrasted results. For instance, Pigeon et al. studied the impact of heritable change in body mass on the growth rate of a population of ungulates and found small effects of evolution (Pigeon et al. 2017). In contrast, several studies in the Soay sheep revealed quite

a strong contribution of phenotypic change to the population growth rate (Pelletier et al. 2007; Ezard, Côté, and Pelletier 2009). Hairston and colleagues, in the paper introducing the Geber method, found that evolutionary change in beak size of the medium ground finch (*Geospiza fortis*) contributed to population growth rate to the same level as seed composition (Hairston et al. 2005). Though the evidence prevents us from generalising, these studies suggest that the importance of eco-evolutionary feedbacks varies across systems.

Finally, we lack empirical evidence regarding the consistency of eco-evolutionary feedback effects in time. The studies listed in the previous paragraph also attempted to quantify the temporal fluctuations of ecological and evolutionary contributions. Pigeon et al. compared effects of phenotypic change on the demography of ungulates across three distinct time periods and found great variation in the strength of evolutionary effects (Pigeon et al. 2017). Pelletier and colleagues showed that the contribution of phenotypic variation to the growth rate of the Soay sheep population fluctuated throughout the time series, and was stronger in low survival years, which hinted at an interaction with environmental conditions (i.e. North Atlantic Oscillations) (Pelletier et al. 2007). Hairston et al. demonstrated that the contribution of the changes in beak size on the population growth rate of (*G. fortis*) was positive but varied considerably in strength (Hairston et al. 2005). Thus, it would seem that the contribution of evolution to ecology, and vice versa, fluctuates in time, and is further potentially contingent on the environmental context (Benthem et al. 2017; Hendry 2019).

Overall, we lack quantitative evidence for eco-evolutionary feedback effects in natural systems, so that it is unclear to what extent they involve indirect effects (e.g. changes in resource levels), how

they unfold and change throughout the time series, and how this varies across species and traits. In this study, we quantify the strength of evolutionary, ecological, and environmental effects and contributions to phenotypic and demographic change in two of the Darwin's finches, *G. fortis* and *G. scandens*, from 1978 to 1991 (Grant and Grant 1993). We assess the consistency of effects and contributions in time to re-build the sequence of ecological, evolutionary, and environmental events that occurred in the system. To do that we use a novel methodology, consisting in fitting neural ordinary differential equations (NODEs, Bonnaffé, Sheldon, and Coulson 2021) to the time series of rainfall and seed supplies, population density, and beak morphology of the finch, to estimate the effect and contribution of environmental, ecological, and evolutionary variables on the ecological and evolutionary change in the two species. By doing so we explore the following questions: (1) is evolutionary change important for demography? (2) In turn, is demographic change a driver of phenotypic change? (3) how do ecological and evolutionary contributions compare to environmental contributions? (4) are feedbacks mediated by changes in resource levels? (5) are these contributions consistent in time? (6) are the effect sizes and temporal patterns of contributions consistent across species and traits within species?

2 Material and Methods

2.1 Method overview

The aim of this study is to infer eco-evolutionary feedback at play in the Darwin's finches system. We use the recently established framework of neural ordinary differential equations (NODEs) to

infer non-parametrically effects and contributions of each state variables of the system to the dynamics of the two species. Effects correspond to the sensitivity of the dynamics to each variable in the system, while contributions provide an estimate of the total amount of variation in the dynamics that is explained by each variable (Hairston et al. 2005).

We consider effects of rainfall and small seed biomass on phenotypic and demographic change in both populations. We allow for effects of medium and large seeds respectively on *G. scandens* and *G. fortis*, as they are specialists of each resource. In each species, we consider effects of population density on phenotypic change, and in turn, effects of the phenotype on population dynamics. We also allow for phenotype-dependence in the dynamics of the phenotypes, and density-dependence in the dynamics of the population. We do not model effects between the two species, as there is evidence that they do not interact directly in the field (Grant and Grant 1993). We further assess the consistency of these effects throughout the time series.

2.2 System

We consider the Darwin's finches system of the Daphne Major island, which consists in two passerine bird species, the medium ground finch, *Geospiza fortis*, and the cactus finch, *Geospiza scandens*, living on a small volcanic island in the Galapagos. They feed mainly on seeds, which can be found in three sizes, small (*Cacabus miersii*), medium (*Opuntia echios*), and large (*Tribulus cistoides*). The medium ground finch feeds predominantly on smaller seeds and will occasionally feed on larger seeds. The cactus finch, feeds predominantly on medium seeds and will occasionally

feed on smaller seeds at low levels of medium seeds.

In 1983, there was an exceptional el Nino event, both in duration and intensity, following a long drought that lasted from 1976 to 1983. The following el Nino events were less strong, and more regular, as they happened every 4 years until 1991. The 1983 el Nino event coincided with a radical change in the seed composition on the island, as well as in the number of individuals and morphology of beaks in the two populations. Large seeds, more endurant to droughts, were depleted, and smaller seeds, which were virtually absent during the drought, became abundant. Coincidentally, the number of individuals in both populations increased drastically, as a result of higher resource levels, and more favourable environmental conditions for breeding. The morphology of beaks changed in accordance with changes in seed composition, as beaks became smaller and more pointed (i.e. narrower) with more abundant small seeds. However, the beak shape of the cactus finch, which is narrower than that of the medium ground finch, became less pointed.

The work of Peter and Rosemary Grant throughout the years established key elements about the mechanism underlying the eco-evolutionary dynamics of the system: (i) the changes in beak size and shape were heritable (Boag 1983), carried-over to the next generations (Grant and Grant 1995), and thereby of evolutionary in nature. (ii) The changes in beak morphology associated at least partly with changes in the survival of individuals, and thereby with the population growth rate (Boag, Grant, and Taylor 1981; Grant and Grant 2000). This sparked interest for the potential for fast feedback effects between ecological and evolutionary change in this system.

We use the time series repository provided by Peter R. and Rosemary B. Grant in their book,

40 years of evolution: Darwin's finches on Daphne Major Island (Grant and Grant 2014). This repository includes time series for the population size, and beak size and shape for both finch species, *G. fortis* and *G. scandens*, as well as resource supplies, namely annual total biomass of small, medium, and large seeds, and yearly rainfall levels on the island. The time series span 16 years, from 1976 to 1991, apart from the time series of medium seed biomass, the collection of which only started in 1979. Population size was estimated by mark capture-recapture survey on the island. Upon capture, individual beak morphology was measured in the form of beak size, depth, and width, and was subjected to a PCA analysis resulting in the identification of two principal components, PC1 beak size, and PC2 beak shape (Grant and Grant 2003). Seed biomass was computed as total annual wet mass of seeds per square meter and were obtained by sampling spatiotemporally randomised quadrats (Grant and Grant 1993). For the sake of conciseness we use the following notation throughout the manuscript: E for yearly rainfall level, R_0, R_1, and R_2 for small, medium, and large seed biomass, N_1 and N_2 for the population size of *G. fortis* and *G. scandens*, P_1 and P_2 for beak size and shape of *G. fortis* and *G. scandens*. E, R_0, R_1, R_2 constitute the environmental variables of the system, N_1 and N_2 the demographic/ecological variables, and P_1, P_2 the phenotypic/evolutionary variables. We transformed the time series of rainfall, small, medium, and large seed biomasses, and population sizes by taking the natural logarithm to prevent negative values from arising in the dynamical models. Each time series was then standardised with respect to its mean and standard deviation to facilitate the fitting process and allow for effects and contributions to be compared within and across the different time series.

2.3 Model specifications

The aim of the modelling approach is to infer the drivers of change in seed supplies, population density, and beak morphology from the time series data. To do this we use NODEs, which is a novel methodology allowing us to infer dynamical processes (i.e. functional representations describing which and how state variables interact and drive the dynamics of the system) non-parametrically from time series data (Bonnaffé, Sheldon, and Coulson 2021). The method relies on approximating the dynamics as non-parametric functions of the variables in the system, using artificial neural networks (ANNs) embedded in an ordinary differential equation (ODE) system (Chen and Chen 1993; Funahashi and Nakamura 1993; Chen et al. 2019; Bonnaffé, Sheldon, and Coulson 2021). The main strength of this methodology is that it is non-parametric, and thus does not require prior knowledge regarding the shape of the dynamical processes, so that it is not subject to incorrect model specifications (Jost and Ellner 2000; Adamson and Morozov 2013). Furthermore, it is likely that the shape of the relationship between some system variables is more complicated than a simple linear function. For instance, the per-capita growth rate of the population may be a nonlinear, bell-shaped, function of the beak morphology in the population, as suggested by previous studies (Hairston et al. 2005). Finally, there may be interactive effects between the system state variables in driving the eco-evolutionary dynamics of the finch population. For example, the effect of the resource on the population per-capita growth rate is likely influenced by beak morphology, as smaller and more pointed beaks are more suitable for picking up small seeds (Grant and Grant 1993).

159 The non-parametric NODE system for *G. fortis* is given as follows

$$
\begin{aligned}
\frac{dR_0}{dt} &= s_1(E, R_0, R_2, N_1, P_1, P_2, \theta_1) \\
\frac{dR_2}{dt} &= s_2(E, R_0, R_2, N_1, P_1, P_2, \theta_2) \\
\frac{dN_1}{dt} &= s_3(E, R_0, R_2, N_1, P_1, P_2, \theta_3) \\
\frac{dP_1}{dt} &= s_4(E, R_0, R_2, N_1, P_1, P_2, \theta_4) \\
\frac{dP_2}{dt} &= s_5(E, R_0, R_2, N_1, P_1, P_2, \theta_5)
\end{aligned}
\tag{1}
$$

160 where dR_0/dt, dR_2/dt, dN_1/dt, dP_1/dt, and dP_2/dt denote the change in small seed log-density
161 (R_0), large seed log-density (R_2), population log-density (N_1), beak size (P_1) and shape (P_2) in
162 continuous time. The functions s are non-parametric functions of the system state. The shapes of
163 the non-parametric functions are controlled by the parameter vectors θ. We did not include a direct
164 interaction between *G. scandens* and *G. fortis* given the differentiation of their ecological niche
165 (Grant and Grant 2003), and limit model complexity. Fitting the NODE system amounts to finding
166 the parameter vectors that best describe the changes in resource, density, and phenotype observed
167 in the time series data. We used the same model structure to analyse the time series of *G. scandens*,
168 except that the variables considered were medium seeds (R_1) instead of large seeds (R_2), to account
169 for the specialisation of *G. scandens* on medium seeds (Grant and Grant 1993), and N_2 instead of
170 N_1, to model population density of *G. scandens*.

171 Each non-parametric functions is an artificial neural network (ANN). ANNs are powerful math-
172 ematical objects that can be trained to approximate the shape of dynamical processes (Funahashi

and Nakamura 1993). For the sake of simplicity, we consider the simplest form of an ANN which contains a single hidden layer, namely a single layer peceptron (SLP)

$$s_1(E,R_0,R_2,N_1,P_1,P_2,\theta_1) = \sum_{i=1}^{I=10} \beta_i f_\sigma \left(\beta_{i0} + \beta_{i1}E + \beta_{i2}R_0 + ... + \beta_{i6}P_2\right) \quad (2)$$

which takes as input the system variables E, R_0, R_2, N_1, P_1, P_2, and output the dynamics of the focal variable considered. The parameter vector θ_1 contain the weights β of the connections in the ANNs. The SLP can be viewed as a weighted sum of basis functions f_σ of the state variables of the system. In this study we consider sigmoid basis functions, as they are commonly used and their capacity to approximate any continuous function is well established theoretically (Funahashi and Nakamura 1993). The number of units in the hidden layer I is chosen to be 10, as this is a commonly used number for systems of that size (e.g. Wu, Fukuhara, and Takeda 2005). More details regarding these models can be found in our previous work (Bonnaffé, Sheldon, and Coulson 2021).

2.4 Model fitting and analysis

We use the fitting approach developed in our previous study (Chapter 3). In this study, we designed a neural network structure specialised in fitting NODEs. The architecture consists of a first layer of neural networks that are specialised in interpolating the state variables, using sinusoid basis functions and by regressing the interpolated function on the time series. Once the interpolations are established, a second layer of neural networks then deals with fitting the NODE equation system

directly to the interpolated dynamics of the states. The NODE system can then be analysed as described in (Bonnaffé, Sheldon, and Coulson 2021). We can recover the effect of each variable on their dynamics by computing the sensitivity of the NODE to a change in each variable. We can also compute the contributions following the Geber method (Hairston et al. 2005), by multiplying the dynamics of a variable by its effect on the dynamics of the focal variable. Finally, we can compute the overall importance of a variable for the dynamics of another one by scoring its relative total contribution, which is obtained by summing its squared contributions across all time steps, and dividing it by the sum of the contributions of all other variables. More details on how to recover these quantities can be found in our previous studies (Chapter 3, Bonnaffé, Sheldon, and Coulson 2021).

We estimate the approximate posterior distribution of the effects and contributions via anchor sampling, which amounts to optimising repeatedly the posterior distribution from different starting points, sampled from the priors (Pearce et al. 2018). As in our previous study, we took 100 samples for each time series, we checked normality and absence of substantial temporal autocorrelation in residuals by visual examination, and we checked the repeatability of the approach by running the fitting procedure a second time. The only departure from our previous approach lies in the fact that we assess the robustness of our results to the choice of standard deviation for the normal priors of the parameters in the networks, whereas in the previous approach, those were optimised as part of the fitting (Chapter 3). This is important given that small prior standard deviations may lead to underfitting, which decreases the variance of perameter estimates and reduces mean estimates

towards 0, while high values may lead to overfitting. Hence, we assess whether the results are qualitatively identical with smaller and larger standard deviation in the prior distributions. All results were found to be robust. Finally, we were not able to perform cross-validation of model results given the small size of the time series considered. This implies that model results may correspond to effects found within the time period of the time series, but they may not extrapolated to later time steps.

3 Results

Eco-evolutionary dynamics of G. fortis

Figure 1 presents the effects and drivers of the environmental, ecological, and evolutionary variables in the *G. fortis* system. All effects are displayed graphically in figure 2.

We find that rainfall is the main positive driver of the dynamics of small seeds (Fig. 1 a, b, red). Large seed and population density contribute negatively to small seed dynamics (Fig. 1 a, b, green, cyan). Small seed density has a positive impact on its own dynamics (Fig. 1 a, b, yellow). We find little evidence for an effect of the traits on small seeds dynamics (Fig. 1 a, b, purple and pink).

The dynamics of large seeds are mainly positively impacted by rainfall and small seed density (Fig. 1 c, d, red and yellow). Large seed density had a small positive effect on its own dynamics (Fig. 1 c, d, green). There is little evidence for an effect of traits and population density on the dynamics

of large seeds (Fig. 1 c, d, cyan, purple, pink).

The dynamics of the population are positively impacted by rainfall (Fig. 1 e, f, red). The positive contributions of traits to population dynamics were comparable to that of rainfall (Fig. 1 e, f, purple and pink). Seed density and population density had a negligible impact on population dynamics (Fig. 1 e, f, yellow, green, and cyan).

The dynamics of beak size are mainly driven by a negative effect of population density (Fig. 1 g, h, cyan), followed by a negative effect of small seed density and rainfall. Interestingly, beak size had a negative effect on its own dynamics (Fig. 1 g, h, purple). We find no effects of large seeds and beak shape on the dynamics of beak size (Fig. 1 g, h, green and pink).

Finally, we find that the dynamics of beak shape are mainly driven by population density and small seed density (Fig. 1 i, j, cyan and yellow). Small seed density has a positive effect on beak shape while population dynamics has a negative effect. We find no support for an impact of other variables.

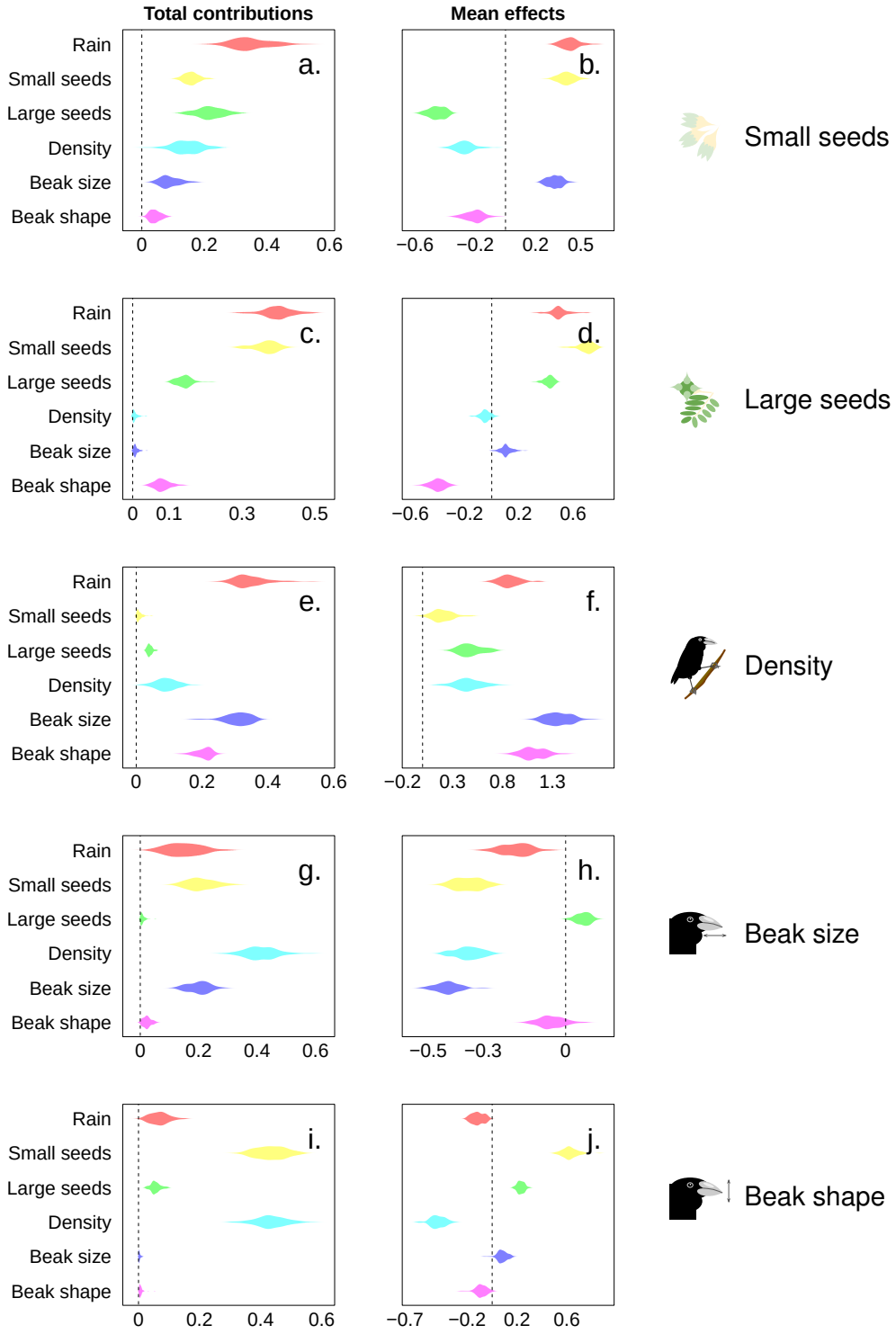

Figure 1: Environmental, ecological, evolutionary effects and contributions in *G. fortis*. Graphs display the total contributions (a, c, e, g, i) and mean effects (b, d, f, h, j) of the state variables, rainfall (red), small (yellow) and large seed biomas (green), *G. fortis* density (cyan), beak size (purple) and shape (pink), on the dynamics of each variable (listed by row). The effects are computed by taking the sensitivity of the NODE approximation of the dynamics with respect to each variable, and then by averaging these effects across the time series. Contributions are computed by multiplying effects by the estimated dynamics of the variable, according to the Geber method (Hairston et al. 2005). Total contributions are calculated as the proportion of the contribution of a given variable to a focal variable across the entire time series, compared to that of all variables combined. The distributions in the graphs correspond to the approximated posterior distributions of the mean effects and total contributions of each variable to the temporal change of a focal variable, estimated by anchor sampling. In all graphs, the dashed line indicates 0.

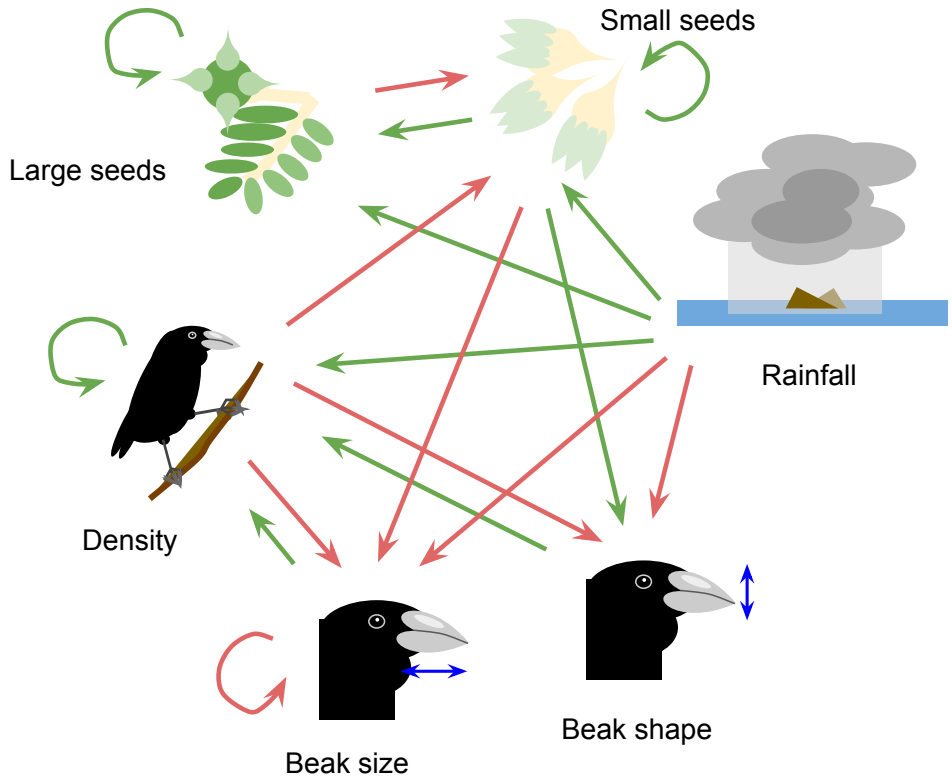

Figure 2: Network of effects underlying the eco-evolutionary dynamics of *G. fortis*. The graph displays the eco-evolutionary dynamics network for *G. fortis*. Arrows correspond to statistically significant effects between variables (green for positive, red for negative). Self arrows correspond to an effect of a variable on itself (e.g. population density-dependence).

Eco-evolutionary dynamics of *G. scandens*

Figure 3 presents the effects and drivers of the variables of the *G. scandens* system. As with *G. fortis*, all effects are summarised graphically in figure 4. We find that the dynamics of small seed are almost solely driven by a positive effect of rainfall (Fig. 3 a, b, red). The dynamics of medium seeds are mostly driven by a positive effect of rainfall (Fig. 3 c, d, red), and a negative effect of beak shape (Fig. 3 c, d, pink). The dynamics of population density (i.e. the per-capita growth rate) are mainly driven by a positive effect of medium seeds (Fig. 3 e, f, green), and rainfall (Fig. 3 e, f, red). We also find a small negative contribution of beak size to the changes in population density (Fig. 3 ,e f, purple). We find that the dynamics of beak size are almost entirely driven by a negative effect of rainfall (Fig. 3 g, h, red). The dynamics of beak shape are driven primarily by a negative effect of rainfall (Fig. 3 i, j, red), and to a lesser extent by positive effects of small seeds, medium seeds, population density, beak size, and beak shape (Fig. 3 i, j, yellow, green, cyan, purple, pink).

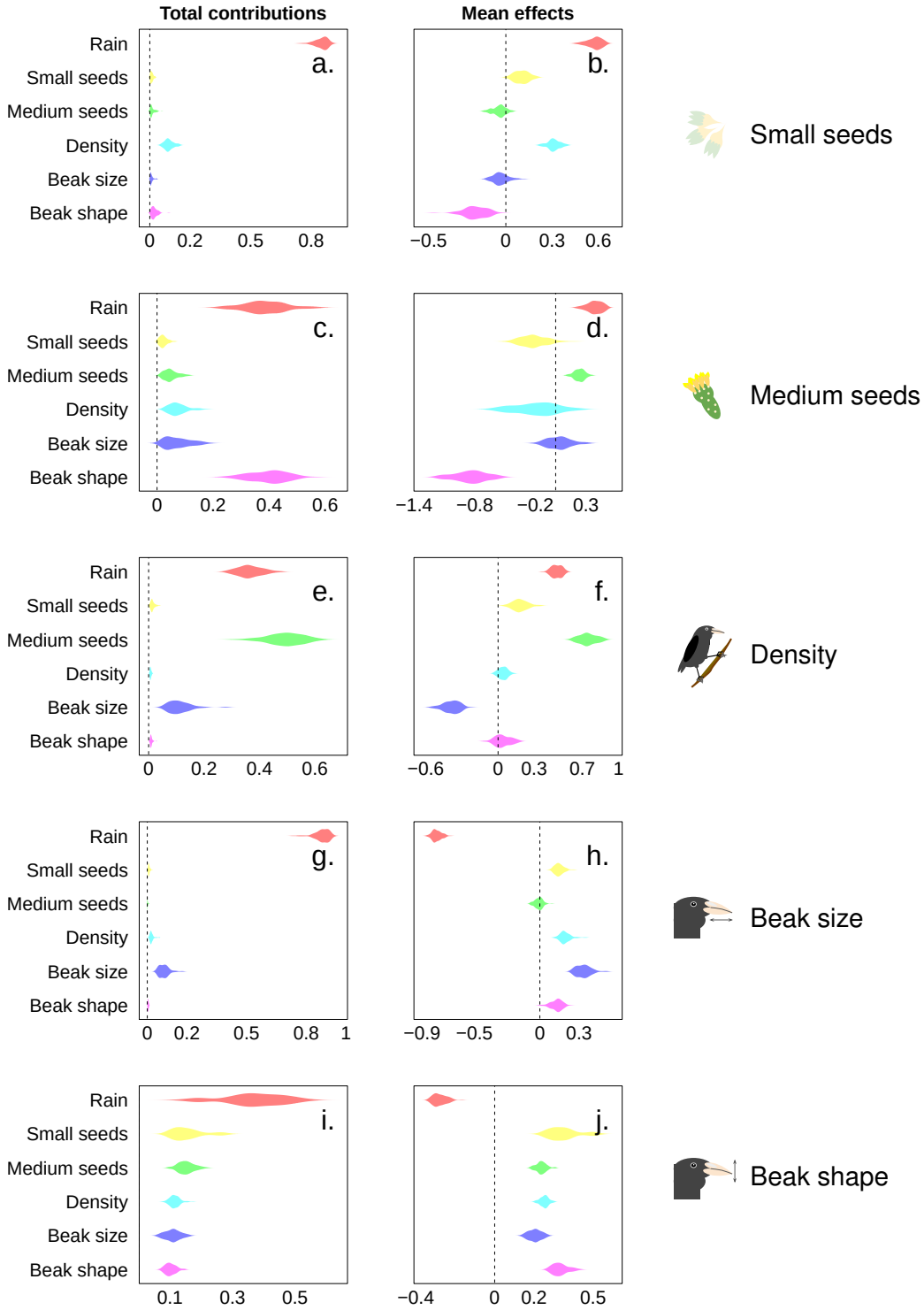

Figure 3: Environmental, ecological, evolutionary effects and contributions in *G. scandens*. Graphs display the total contributions (a, c, e, g, i) and mean effects (b, d, f, h, j) of the state variables, rainfall (red), small (yellow) and medium seed biomas (green), *G. scandens* density (cyan), beak size (purple) and shape (pink), on the dynamics of each variable (listed by row). The effects are computed by taking the sensitivity of the NODE approximation of the dynamics with respect to each variable, and then by averaging these effects across the time series. Contributions are computed by multiplying effects by the estimated dynamics of the variable, according to the Geber method (Hairston et al. 2005). Total contributions are calculated as the proportion of the contribution of a given variable to a focal variable across the entire time series, compared to that of all variables combined. The distributions in the graphs correspond to the approximated posterior distributions of the mean effects and total contributions of each variable to the temporal change of a focal variable, estimated by anchor sampling. In all graphs, the dashed line indicates 0.

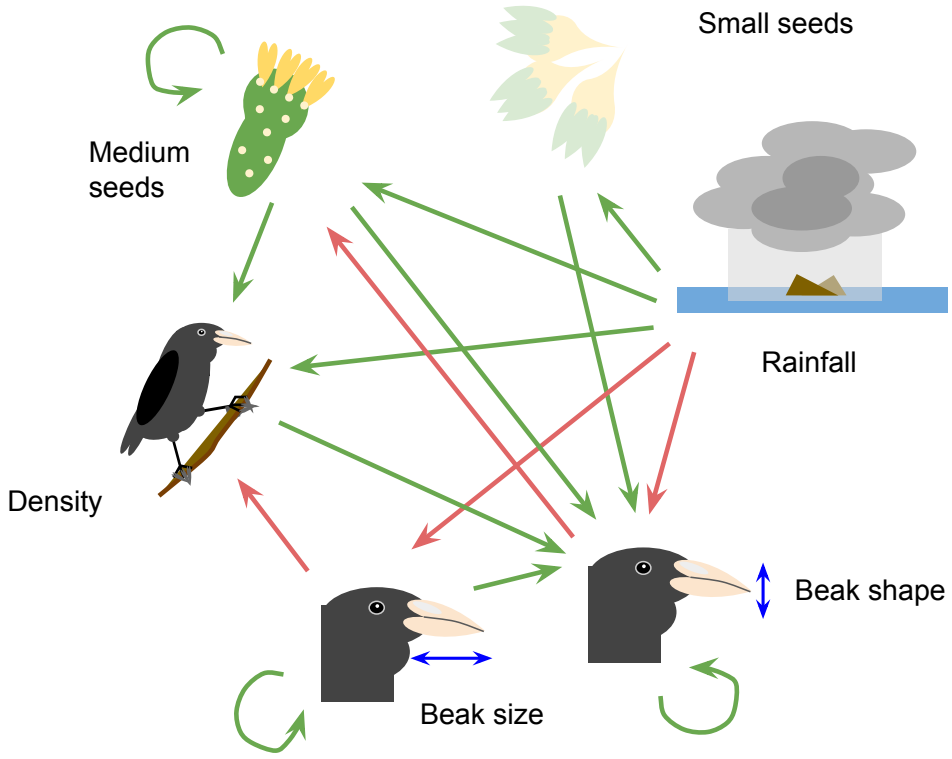

Figure 4: Network of effects underlying the eco-evolutionary dynamics of *G. scandens*. The graph displays the eco-evolutionary dynamics network for *G. scandens*. Arrows correspond to statistically significant effects between variables (green for positive, red for negative). Self arrows correspond to an effect of a variable on itself (e.g. population density-dependence).

Temporal consistency of effects in *G. fortis*

Figure 5 and 6 presents the temporal consistency of effects underlying the ecological and evolutionary dynamics of *G. fortis* revealed by the NODE analysis. Effects underlying the population growth rate are mostly consistent throughout the time series except for a reduction of effect size during the most stable part of the time series (Fig. 5, effects, time steps 1-4). We find that the population growth rate is initially mainly altered by changes in beak size (Fig. 5, contributions, time steps 0-2, blue line), then by rainfall (time steps 3-6, red line), then by the two traits (6-7, blue and purple lines), and by rainfall again for the remainder of the time series (time steps 7-10, red line). The effects of the variables on the dynamics of beak shape are mostly consistent in spite of an increase in effect size around time step 6 (Fig. 6, effects). The dynamics of beak shape is mostly driven by changes in small seed density and population density (Fig. 6, contributions, time steps 0-6, yellow and blue lines), and in later stages of the time series, almost solely by population density (Fig. 6, contributions, blue line).

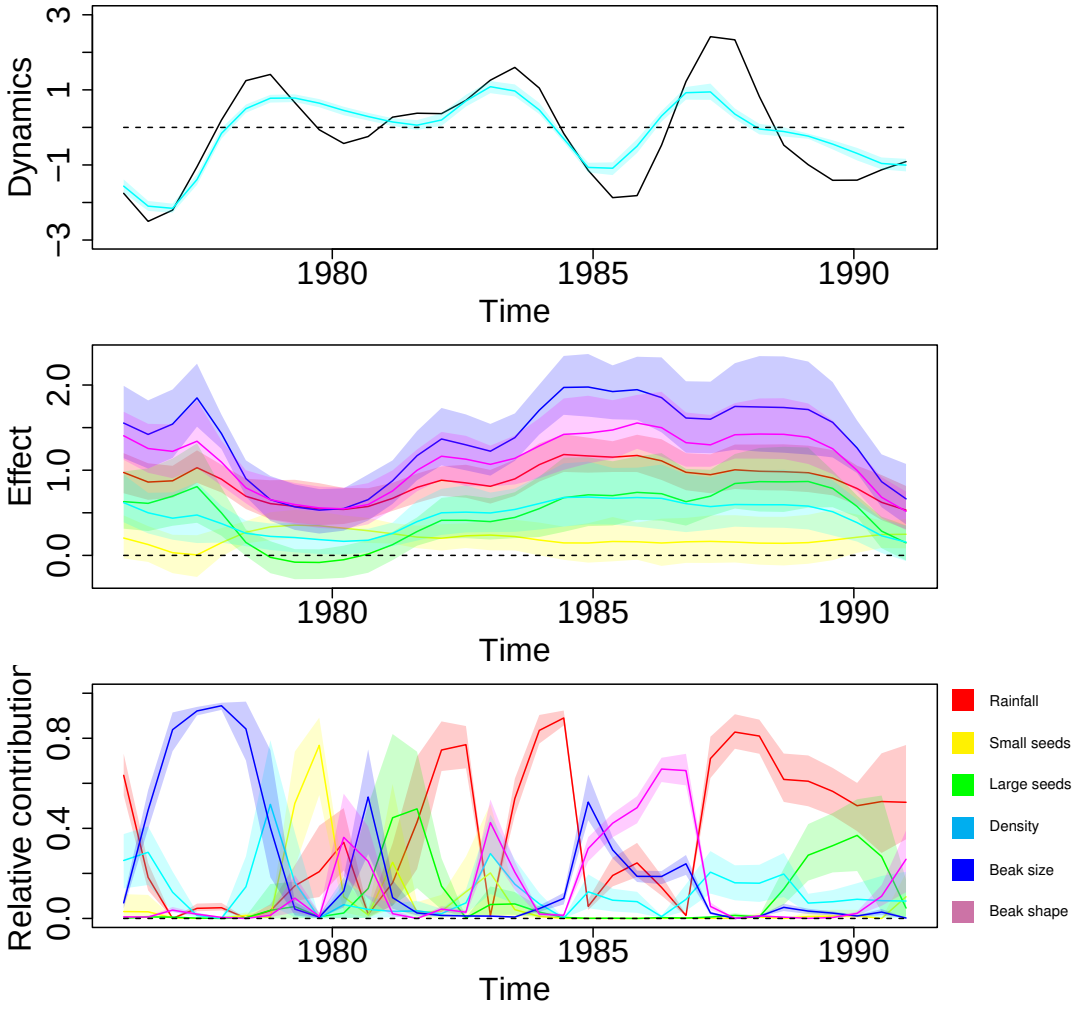

Figure 5: Drivers of eco-evolutionary dynamics of *G. fortis* density. Row (1) presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row (2) presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row (3) presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

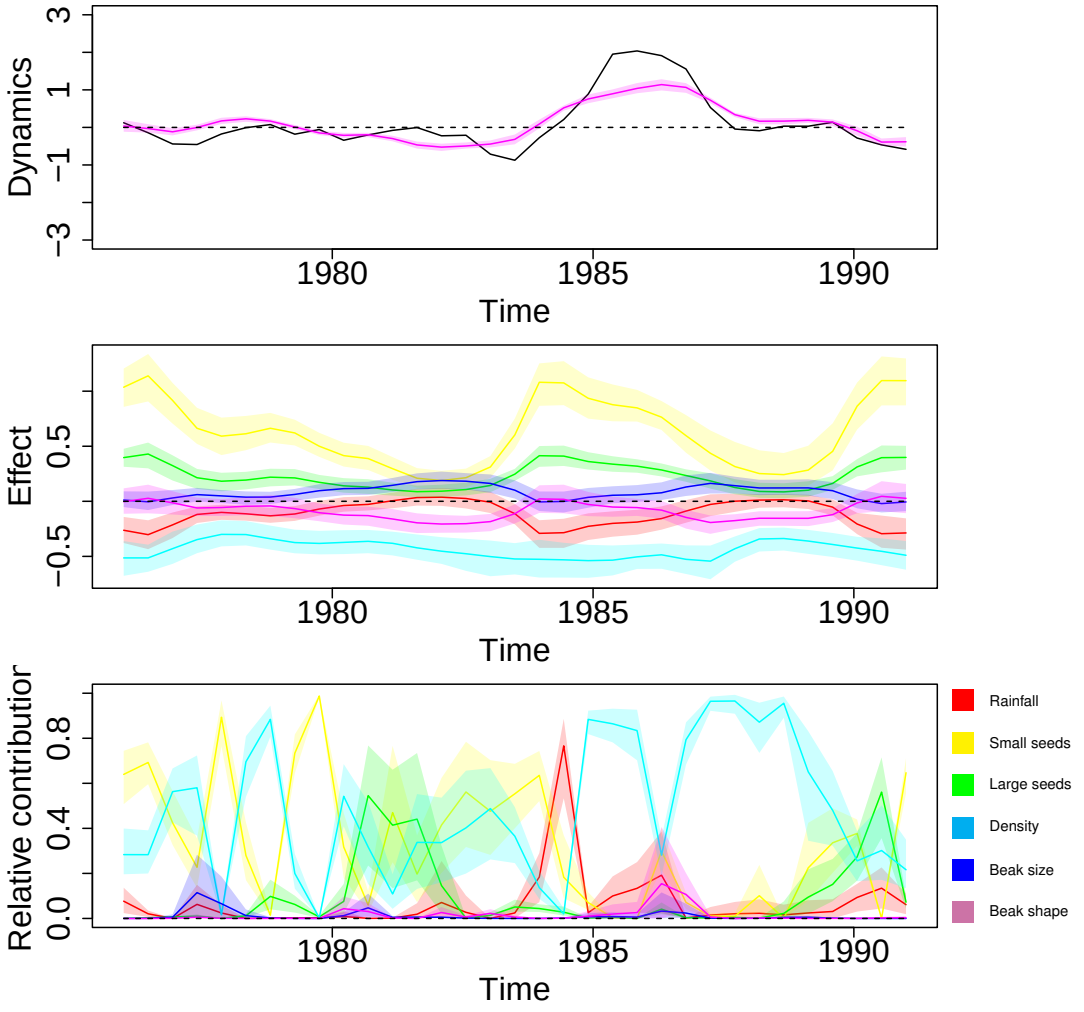

Figure 6: Drivers of eco-evolutionary dynamics of *G. fortis* beak shape. Row (1) presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row (2) presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row (3) presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

4 Discussion

In this study, we inferred the environmental, ecological, and evolutionary drivers of eco-evolutionary dynamics of two of Darwin's finches, the medium ground finch (*G. fortis*), and the common cactus finch (*G. scandens*). We used NODE models to estimate non-parametrically the effect of each variable on the dynamics of the other, as well as its relative contribution to the total change observed in each time series. We find a dominating effect of rainfall in driving the dynamics of all variables. The structure of eco-evolutionary feedbacks between population density, resource levels, and beak morphology, differed between the two species. In *G. fortis*, we found two types of feedbacks, one direct feedback between population density and changes in beak shape and size, but also a feedback mediated by an effect of population density on resources, small seeds, which in turn influenced further beak evolution. In *G. scandens*, we found only evidence for a direct feedback between resource level, namely medium seeds, and beak shape. These results support the general view in eco-evolutionary dynamics that feedback effects between ecology and evolution can be comparable in strength to environmental effects. Our findings also suggest that indirect feedback effects involving resource levels may be common in nature and comparable in strength to direct effects. Our results also show considerable variation in feedback structure across two closely related species, suggesting great variability in feedback structure across species and systems. Finally, our study supports a considerable amount of context-dependence in feedback effects, given the temporal variation in effect size that we find across the time series. We discuss below our main findings and differences in feedbacks between these two species in light of the literature.

Eco-evolutionary dynamics of *G. fortis*

We find that the dynamics of the population of *G. fortis* are mostly driven by rainfall. This was initially noted by the Grants, and later confirmed by Hairston and Beausoleil (Grant and Grant 1993; Hairston et al. 2005; Beausoleil et al. 2019). These studies demonstrated a positive effect of rainfall on population dynamics, via a positive effect on breeding (Grant and Grant 1993). This would also explain why we find no evidence of an impact of seed supplies on the growth rate of *G. fortis*. The effect of seed supplies may already be accounted for by rainfall (Beausoleil et al. 2019).

Beak morphology impacted strongly the dynamics of the *G. fortis* population. Hairston already found a positive effect of the dynamics of beak size on population growth but failed to identify one of beak shape, due to the low statistical power imposed by the short time series (Hairston et al. 2005). Studies by the Grants demonstrated that the link between beak shape and fitness was inconsistent, possibly in line with environmental variation disrupting selection (Grant and Grant 2000). This was recently confirmed by Beausoleil, who showed that indeed, variation in climatic variables, such as rainfall, disrupted the direction of selection on beak shape, and thereby the relationship between fitness and beak morphology (Beausoleil et al. 2019). However, these studies were performed at the individual-level, and considered each year separately. The fact that we find a clear effect of both morphological trait in our study suggests that considering the time series as a whole may help unveil processes otherwise hard to detect. Overall, this result confirms the view that feedback effects can be as important as environmental effects (Hairston et al. 2005; Ezard,

Côté, and Pelletier 2009).

In turn, we find that the dynamics of the traits of *G. fortis* are mostly driven by population density, rainfall, and small seed density. The positive effect of small seeds on beak shape and its negative effect on beak size are consistent with the idea that small seeds favour smaller and more pointed beaks (Grant and Grant 1993). Yet, as far as we know, no work to date has demonstrated a dominant impact of population density and rainfall on beak evolution in *G. fortis*. This result is indirectly supported by Beausoleil who evidenced a strong link between climatic variables and selection on beak morphology (Beausoleil et al. 2019).

Eco-evolutionary dynamics of *G. scandens*

As for *G. scandens*, we find that population dynamics are mostly driven by rainfall and medium seeds. Similarly, the evolution of beak morphology was mainly driven by rainfall, and in the case of beak shape, by medium seeds. These results are not surprising considering that *G. scandens* feeds almost exclusively on medium seeds (Grant and Grant 1993), contrary to *G. fortis*, who is more of a generalist. We do not find evidence for an effect of beak morphology on population growth. In line with this result, the few studies that assessed fitness consequences of beak morphology in *G. scandens* failed to find any consistent effects (Grant and Grant 2000). To our knowledge, our study is the first to evidence an eco-evolutionary feedback between medium seed density and beak shape in *G. scandens*, possibly in line with a study bias in favour of *G. fortis*.

Comparison of *G. fortis* and *G. scandens*

One of the striking differences between *G. fortis* and *G. scandens* is the absence of a connection between trait evolution and demography in *G. scandens*. As stated before, other studies also found little evidence for such a link in *G. scandens* compared to *G. fortis* (Grant and Grant 2000; Hairston et al. 2005; Beausoleil et al. 2019). We think it intriguing to find changes in the traits that are explainable by ecological and environmental factors, but yet do not have observable consequences on population dynamics. This questions the nature of the evolutionary process at play, and the potency of fitness gradient models for explaining evolution in natural systems. But most importantly, this finding hence suggests the existence of cryptic eco-evolutionary feedbacks in nature, between environmental and evolutionary variables, which may not have apparent demographic consequences. As far as we are aware, no such idea has been considered before in the context of eco-evolutionary feedbacks, though this is a natural implication of cryptic evolution (Kinnison, Hairston, and Hendry 2015).

Importantly, we find eco-evolutionary feedbacks between the resource and the traits in both species. Only few studies have empirically demonstrated such feedbacks in a natural setting, though resource density is viewed as an important component of feedbacks (Govaert et al. 2019). Most study focus on detecting density-dependence in evolutionary change (e.g. Reznick et al. 2019), or selection in demography (e.g. Grant and Grant 2000; Hairston et al. 2005; Pigeon et al. 2017). The effect of the ecological and evolutionary dynamics of the population on resources are still rarely considered in the same study. Especially in the finch system, only one study, to our knowledge, has investigated the impact of beak evolution on the evolution of seed defense (Carvajal-Endara et al.

2020). Our study confirms that eco-evolutionary feedbacks involving resources are important and ubiquitous in nature, as already suggested by recent work on guppies (Simon et al. 2017).

Our study also reveals temporal variation in the effects in both species system. This points to complex interactions between the variables, and thereby high context-dependency of eco-evolutionary processes. This adds to studies on the finch that demonstrated inconsistent links between fitness and beak morphology, potentially in line with environmental context-dependence (Grant and Grant 2000; Beausoleil et al. 2019). This adds to studies in ungulates that found that the contribution of evolution to population growth varied across different periods (Pigeon et al. 2017). Our works provides an example of how these effects vary in time as a result of changes in the state of the system. We need more studies to understand the importance of context-dependence in eco-evolutionary dynamics, by considering for instance interactions between density, resources, environmental variables (Brunner et al. 2019).

Overall, we found substantial differences in the feedback architecture underlying the eco-evolutionary dynamics of these two closely related species. This supports the idea that we should expect a high diversity of feedback architectures in natural systems (Hendry 2019; Brunner et al. 2019). Our study, by providing a complete view of feedbacks at play in a system featuring multiple species and traits, is a first step towards unveiling this diversity (e.g. Becks et al. 2010; Becks et al. 2012). An intriguing prospect would be to study the consistency of feedback structures across replicated systems in controlled environments, to establish a baseline for our expectation regarding feedback repeatability and diversity.

366 Characterising this diversity is key to generalising eco-evolutionary dynamics across systems. This
367 can be done by identifying ubiquitous components of dynamics, for instance, consistent species
368 interactions, or environmental conditions that favour a strong evolutionary response. This may
369 have further implications for population management, or anticipating climate change, where our
370 understanding of other systems would allow us to gage the importance of evolution for the viability
371 of a system under threat (Benson et al. 2016). We are progressively incorporating complexity on a
372 higher level, for instance, by considering eco-evolutionary community dynamics holistically. The
373 hope with machine learning techniques, such as the one developed here, is that they would allow
374 us to continue on this path without sacrificing complexity in lower-levels.

375 **Other dynamical effects**

376 We also find surprising effects outside of the feedbacks considered in the previous paragraphs.
377 First, we find positive intra-specific density-dependence in *G. fortis*, which indicates that the pop-
378 ulation tends to increase more at high density. To our knowledge, this result is novel, as intra-
379 specific density-dependence in *G. fortis* has received little attention. Given the small population
380 size, this effect is potentially the result of a benefit in mating and breeding success at higher den-
381 sities. We also find evidence for positive intra-specific density-dependence in the dynamics of the
382 small and large seeds. This suggests that higher seed biomass associates with a higher increase in
383 seed biomass in subsequent years, potentially in line with higher survival of plants to predation.
384 We also found that small seed biomass had a positive effect on large seed dynamics, while large
385 seed biomass had a negative impact on small seed dynamics. This may be explained by a competi-

tive interaction between these two species. Interestingly, this interaction is found to be inconsistent with the observation, made by the Grants, that *Cacabus* (small seeds) could "smother" *Opuntia* (large seeds) (Grant and Grant 1993).

Second, we found evidence for self-effects in phenotype dynamics. In *G. fortis*, beak size had a negative effect on its own dynamics. This means that phenotypic change in *G. fortis* tended to decelerate as beak size increased. This suggests the existence of structural constraints on beak size, developing larger beaks might come at higher development and metabolic costs (e.g. Brown et al. 2004). In *G. scandens*, we only find a small positive effect of beak shape on its own dynamics. This suggests that the reduction of beak pointedness in the cactus finch tended to decelerate over time. In addition to structural constraints (see above), this effect could be explained by a reduction of genetic variation over time, which would constrain the evolution of beak morphology. Yet, evidence for genetic variation constraints on evolution is unlikely in this system (Keller et al. 2001).

Prospects

There are aspects of the evolutionary response of the finch that our study does not address. First, we modelled implicitly interactions between variables. We hence did not show which variables were accounting for a change in the effects across the time series. For instance, it is likely that seed supplies are conditioning the strength of the effects of traits on demography and vice versa (Hairston et al. 2005). An interesting prospect could be to explore these interactions, by looking at the Hessian of the system, namely the sensitivity of the effects to each variable.

Additionally, our simple NODE model does not allow for lag effects involving variables not ac-

406 counted for in this system. For instance, there may be delayed effects of seeds on population
407 growth mediated by changes in the age- and size-structure of the population (Grant and Grant
408 2000). Another prospect could hence be to either add latent variables, which act as stepping stones
409 to propagate effects in time, or to analyse the second or third order derivatives of the dynamics of
410 the variables in time, which would unveil delayed effects.

411 Finally, our approach hints at effects of variables and interactions but it does not reveal specific
412 mechanisms. One fascinating prospect would be to compare the consistency of effects inferred
413 by NODEs with state of the art mathematical theory (e.g. Patel, Cortez, and Schreiber 2018; Lion
414 2018; Lion et al. 2018; Govaert et al. 2019). In particular in this system, our NODE model provides
415 an approximation of the selection gradient, that is the sensitivity of population growth to a change
416 in beak size and shape. By combining the Geber method and the Price equation (Ellner, Geber, and
417 Hairston 2011), we could compute how much of phenotypic change is explained by the selection
418 gradient approximated non-parametrically by the NODE.

419 **Conclusion**

420 We inferred the drivers of eco-evolutionary dynamics of *G. fortis* and *G. scandens* with NODEs.
421 The environmental variable, rainfall, was the most influential variable as it affected the dynamics of
422 the finch and seed supplies. We found a strong coupling between beak evolution and demography
423 in *G. fortis*, but not in *G. scandens*. In both species, seed supplies played a crucial role in the
424 evolutionary dynamics of beak morphology. This shows variation in eco-evolutionary feedback
425 structure in two closely related species, on the same island. Our study hence confirms the strength

of the coupling between ecological and evolutionary variables, and further hints at a high degree of context-dependence in eco-evolutionary processes.

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Data accessibility

All data and code will be made fully available at https://github.com/WillemBonnaffe/NODER/D-Finch.

Statement of authorship

Willem Bonnaffé designed the method, performed the analysis, wrote the manuscript; Tim Coulson led investigations, provided input for the manuscript, commented on the manuscript. Ben C. Sheldon led investigations, provided input for the manuscript, commented on the manuscript.

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541 lution drives ecological dynamics in a predator – prey system”. In: *Nature* 424.July, pp. 303–
542 306.

5 Supplementary

A Temporal variation in effects and contributions in *G. fortis*

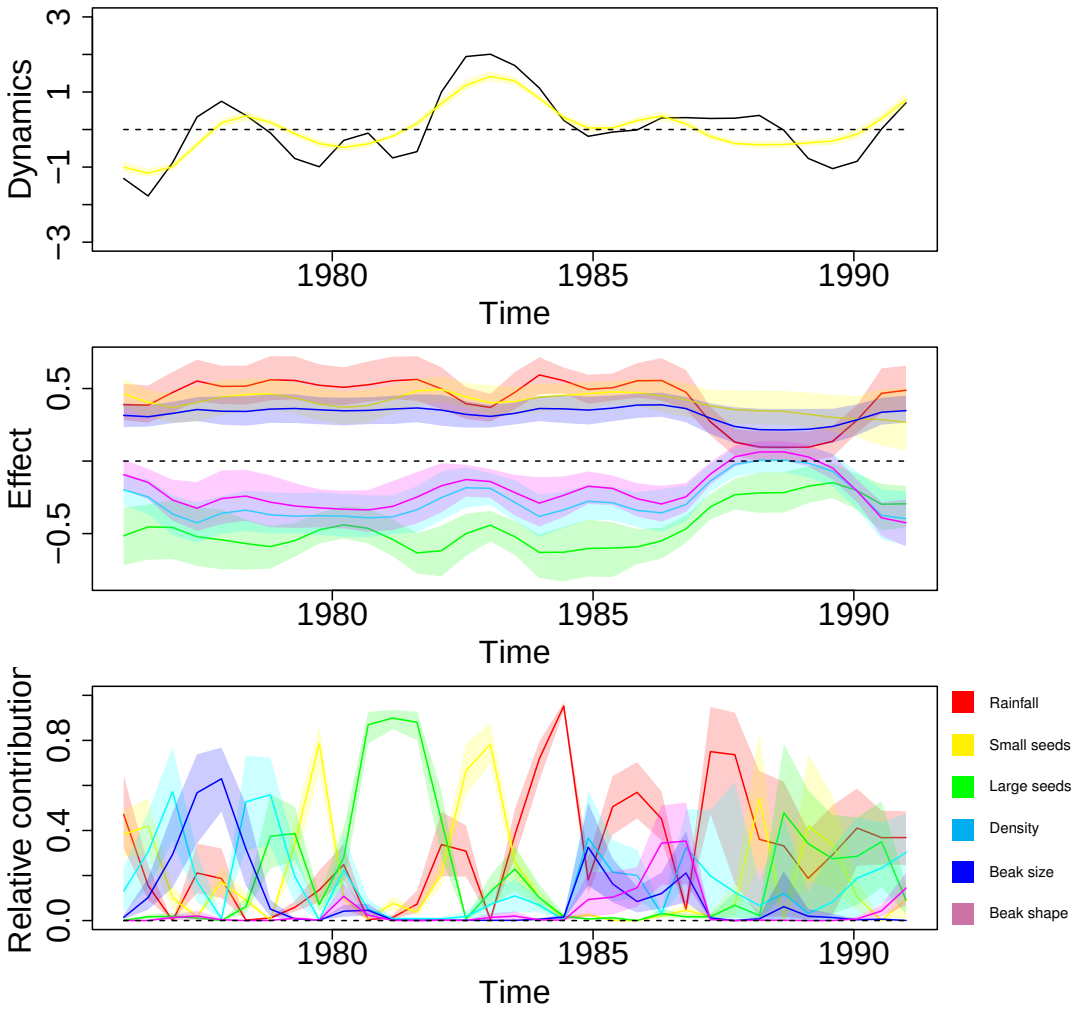

Figure S1: Temporal variation in effects and contributions to the dynamics of small seed density. Row 1 presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row (2) presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row (3) presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

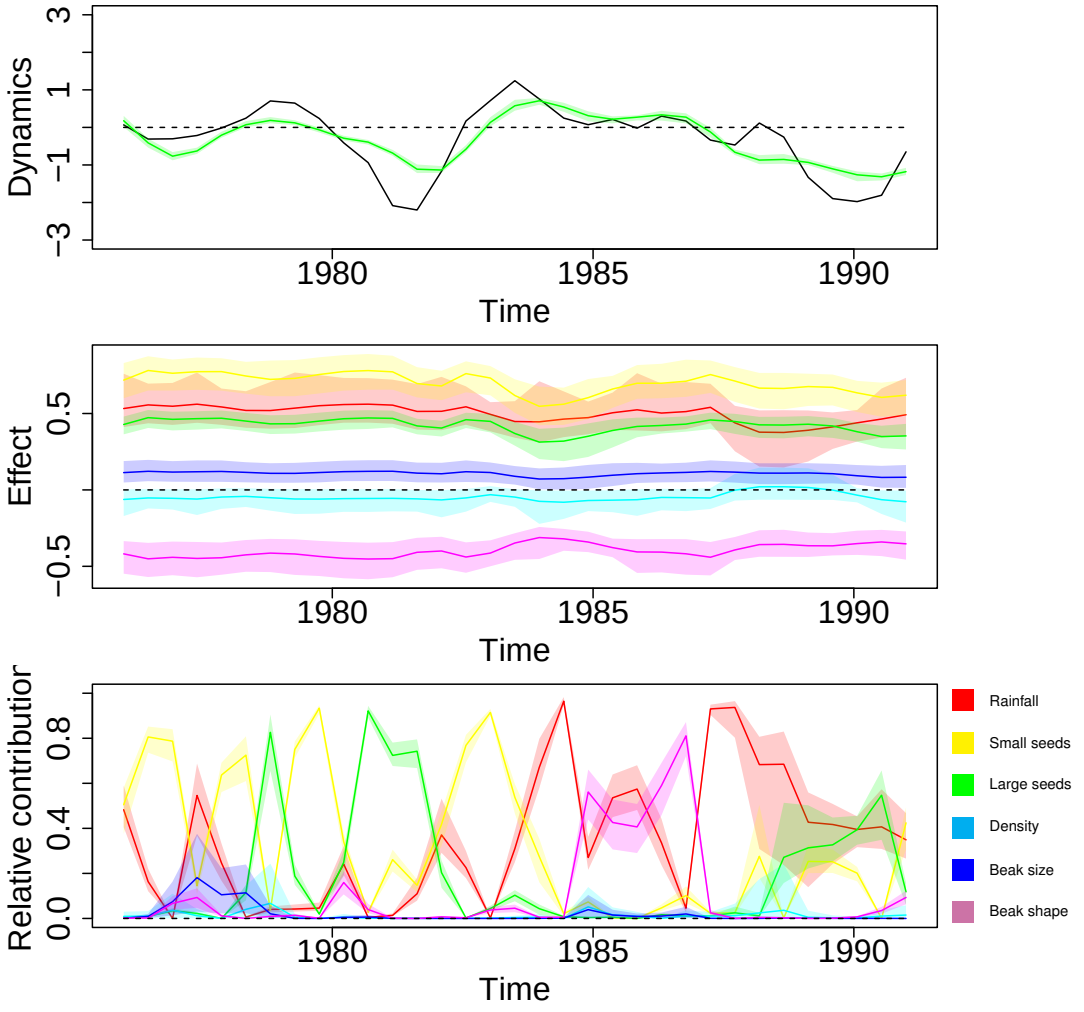

Figure S2: Temporal variation in effects and contributions to the dynamics of large seed density. Row 1 presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row 2 presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row 3 presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

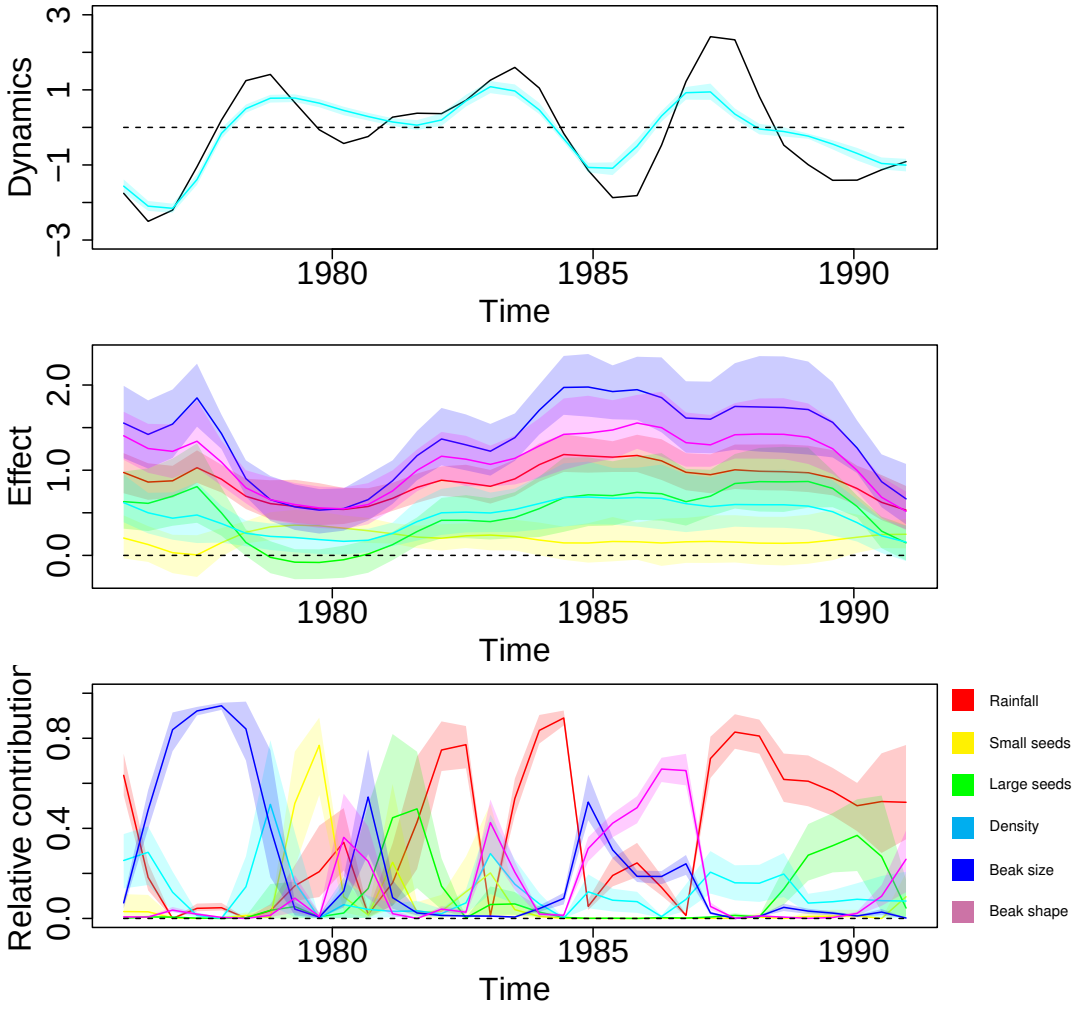

Figure S3: Temporal variation in effects and contributions to the dynamics of *G. fortis* density. Row 1 presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row 2 presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row 3 presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

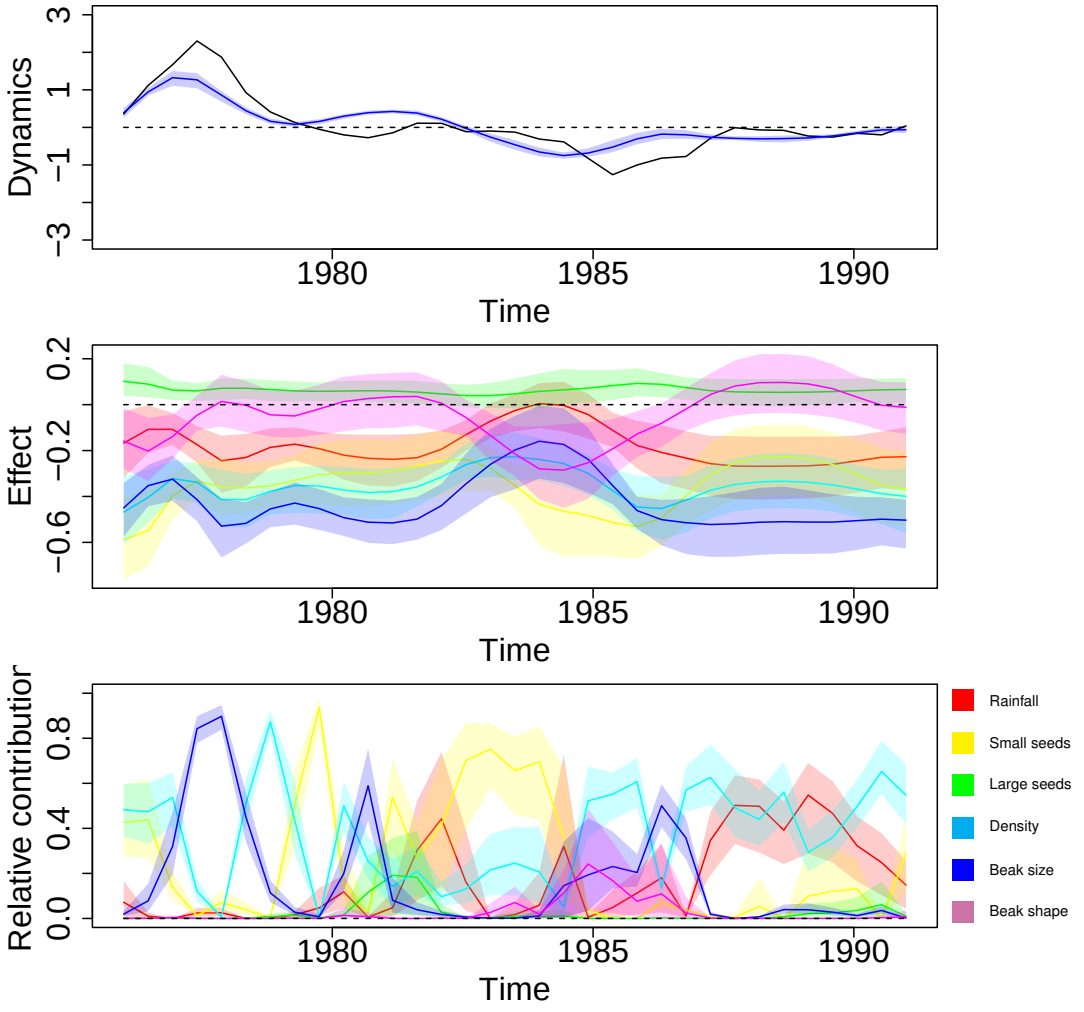

Figure S4: Temporal variation in effects and contributions to the dynamics of *G. fortis* beak size. Row 1 presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row 2 presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row 3 presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

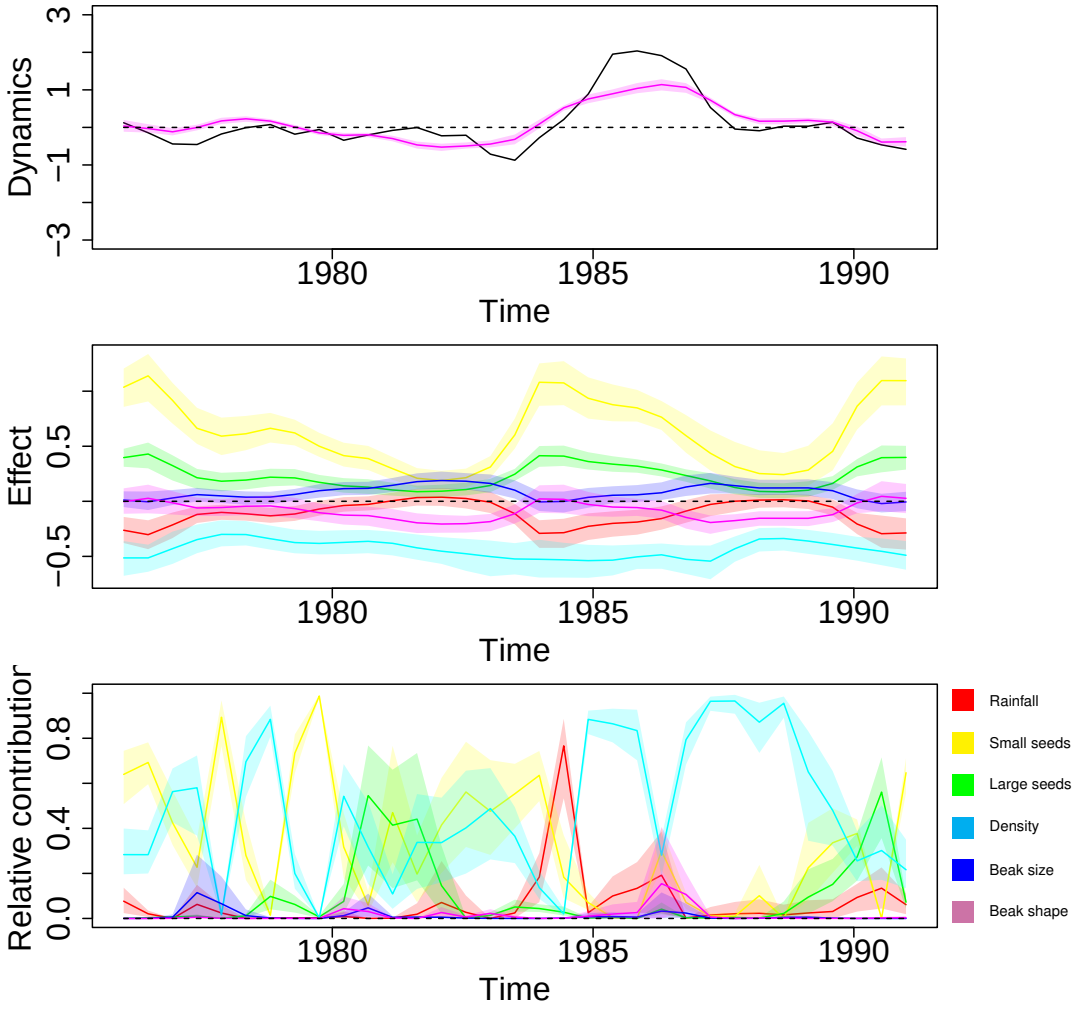

Figure S5: Temporal variation in effects and contributions to the dynamics of *G. fortis* beak shape. Row 1 presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row 2 presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row 3 presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

B Temporal variation in effects and contributions in *G. scandens*

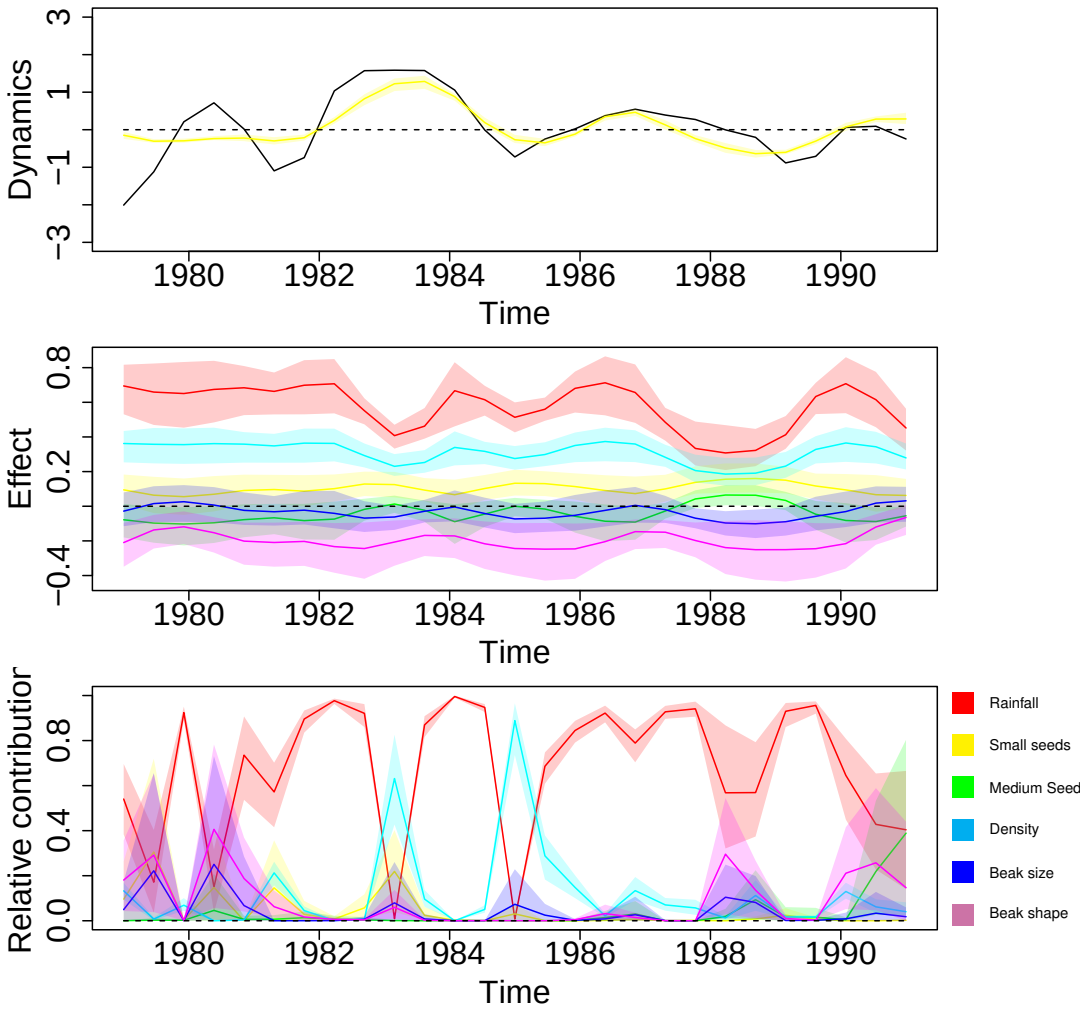

Figure S6: Temporal variation in effects and contributions to the dynamics of small seed density. Row 1 presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row 2 presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row 3 presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

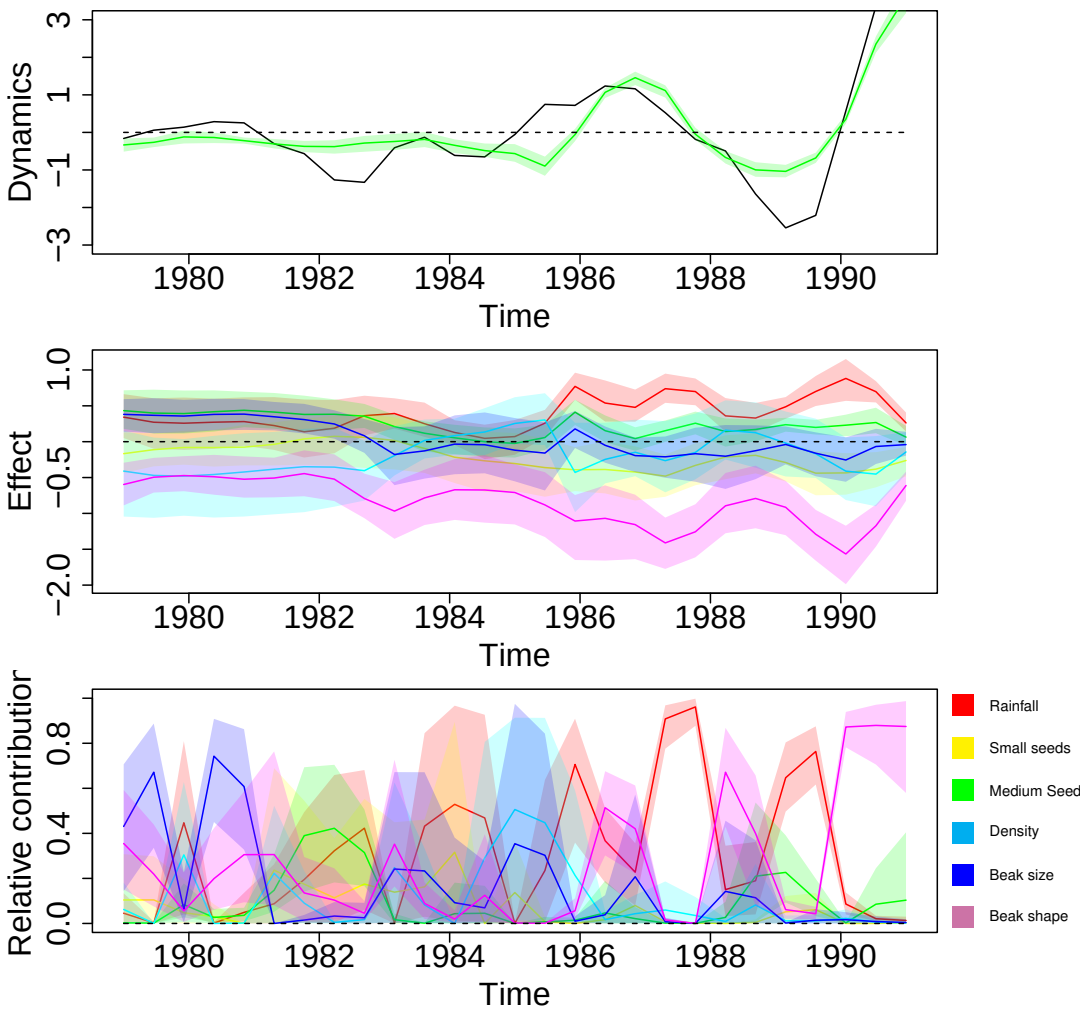

Figure S7: Temporal variation in effects and contributions to the dynamics of medium seed density. Row 1 presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row 2 presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row 3 presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

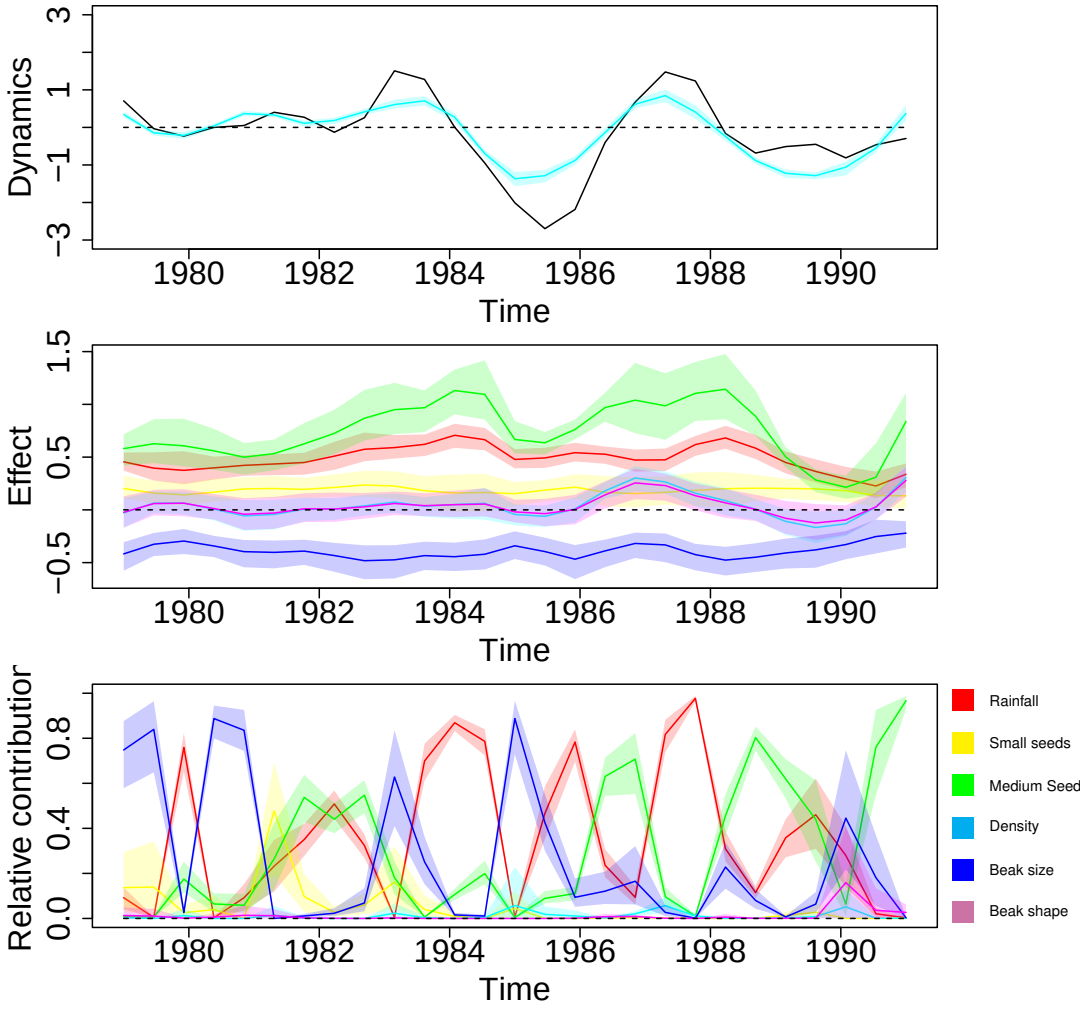

Figure S8: Temporal variation in effects and contributions to the dynamics of *G. scandens* density. Row 1 presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row 2 presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row 3 presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

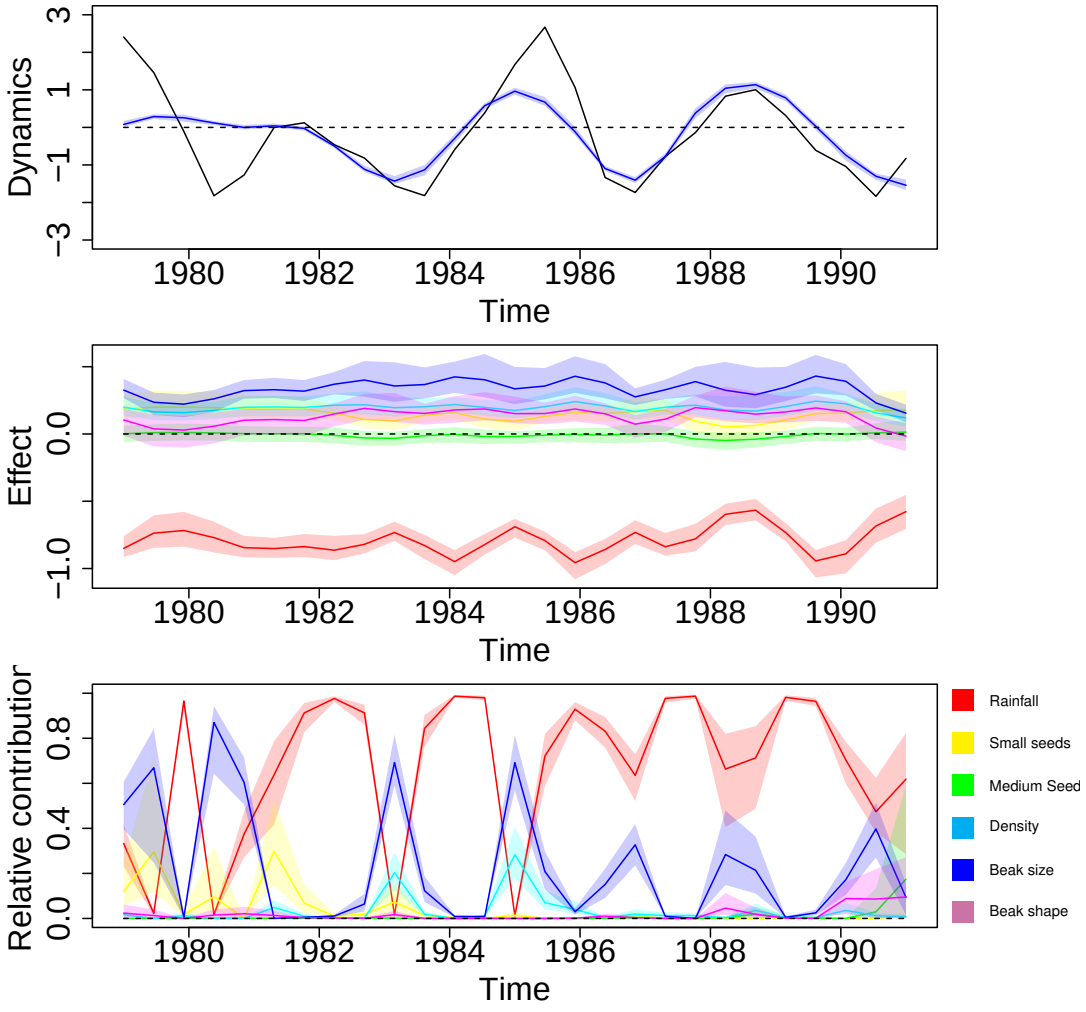

Figure S9: Temporal variation in effects and contributions to the dynamics of *G. scandens* beak size. Row 1 presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row 2 presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row 3 presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

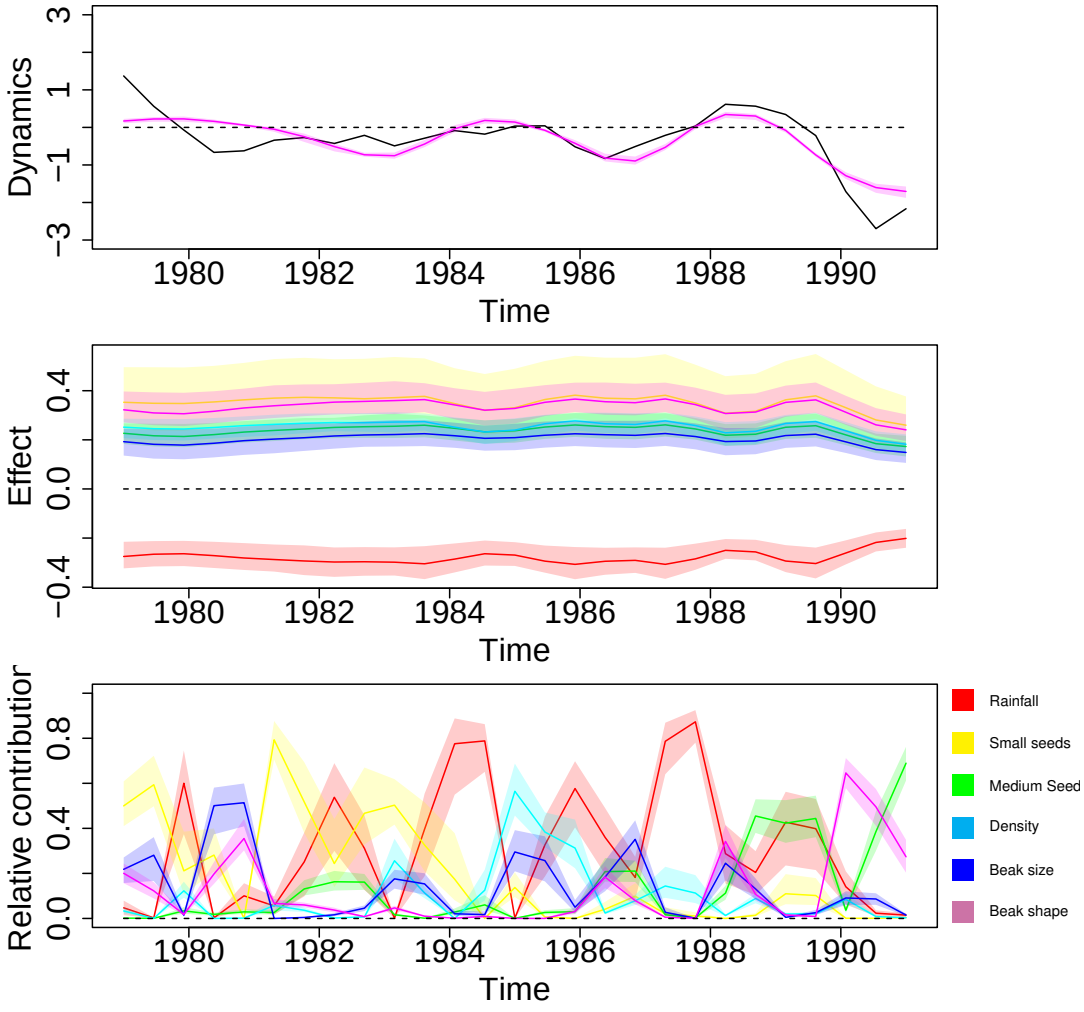

Figure S10: Temporal variation in effects and contributions to the dynamics of *G. scandens* beak shape. Row 1 presents the change in state at each time step, where the black line is the change derived from the interpolated data and the coloured line is the NODE approximation. Row 2 presents the effect of each variable on the dynamics of the focal variable, obtained by computing the sensitivity of the NODE approximation with respect to each variable. Row 3 presents the relative contribution of each variable to the dynamics of the focal variable, obtained by multiplying its effect by its dynamics, compared to the contribution of other variables.

Part V

Chapter 5: General discussion

General discussion

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Statement of authorship: Willem Bonnaffé wrote the manuscript; Tim Coulson commented on the manuscript. Ben C. Sheldon commented on the manuscript.

1 General discussion

Ecology and evolution were thought to operate on different time scales. Evolutionnary change would operate in the course of millions of years, while ecological change would happen within an organism's lifetime. For this reason, ecological and evolutionnary change were studied independently on one another (Fussmann, Loreau, and Abrams 2007; Pelletier, Garant, and Hendry 2009). More recently, empirical evidence from two iconic systems, the Guppy fish in Trinidad and the Darwin's Finches in the Galapagos, demonstrated that evolution could proceed fast enough to interplay with ecological change (Reznick, Bryga, and Endler 1990; Boag, Grant, and Taylor 1981; Grant and Grant 1993). This gave birth to the concept of eco-evolutionary feedback effects, which correspond to the pathways through which ecological change affects evolutionary change, and vice versa (Pimentel 1968; Pelletier, Garant, and Hendry 2009; Post and Palkovacs 2009; Schoener 2011). Though feedbacks have been extensively studied in theoretical work, there is still a shortage of quantitative evidence from real systems providing a complete view of all the effects that may tie ecological variables to evolutionary variables (Hendry 2019; De Meester et al. 2019; Brunner et al. 2019). This stems from the complexity and uncertainty surrounding the mechanisms for feedbacks, which hinders the formulation of mathematical hypotheses and makes for a burdensome comparison of models to real data. This leaves some key questions in the field of eco-evolutionary dynamics unanswered. What is the relative strength of indirect feedback effects, for instance, mediated by changes in resources, compared to direct effects, and to environmental effects (Hendry 2019)? Are feedback effects consistent in time, or do they fluctuate due to context-dependence

(Brunner et al. 2019)? Are feedbacks conserved across similar traits and species (De Meester et al. 2019)? And ultimately, how important and ubiquitous are feedbacks in nature (Schoener 2011; Ellner, Geber, and Hairston 2011)?

To answer these questions, we need specialised methods to infer feedback architecture in systems that undergo rapid evolution. Feedbacks are studied through theoretical and empirical approaches. Theoretical approaches mainly rely on ODE models to learn the eco-evolutionary dynamics enforced by different feedback architectures (e.g. Ellner, Geber, and Hairston 2011; Lion et al. 2018; Lion 2018; Patel and Bürger 2019; Cortez, Patel, and Schreiber 2020). The main empirical approach to quantify feedback directly from time series data has consisted in the Geber method, which quantifies the importance of the impact of evolutionary change on the growth of populations (Hairston et al. 2005, e.g. Ezard, Côté, and Pelletier 2009; Ellner, Geber, and Hairston 2011; Pigeon et al. 2017). Yet, too few studies combined these two approaches, by using the Geber method to quantify feedbaks in theoretical models fitted to real time series data (but see Van Velzen and Gaedke 2017). These approaches also suffer from the lack of prior knowledge regarding the potential mechanisms underlying feedbacks, meaning that feedback effects thereby inferred may be contingent on the choice parametric structure used to model them (Jost and Ellner 2000; Adamson and Morozov 2013). Finally, most studies only report effect size of feedbacks, but variation in feedback effects have received less attention (Hendry 2019).

In this thesis, we make steps towards addressing these methodological limitations to provide quantitative evidence for feedbacks in real systems. In the first chapter we build upon latest developments

in Bayesian statistics and machine learning applied to dynamical systems modelling (Chen et al. 2019; Pearce et al. 2018). We improve current methods for quantifying feedbacks in three ways. First, we merge the Geber method with ODE models, to quantify feedback effects in a consistent eco-evolutionary dynamics model. Second, we develop a non-parametric framework to infer feedback effects where mechanistic knowledge is lacking. Finally, we embed the framework in a Bayesian context to quantify uncertainty in feedback effects given on time series data collected in real systems. The framework, called neural ordinary differential equation (NODEs), provides a method suitable for quantifying the coupling between environmental, ecological, and evolutionary variables from time series data, where mechanistic knowledge on dynamical processes is lacking (i.e. functional representations describing which and how state variables interact to determine the dynamics of the system).

In the second chapter, we apply the NODE methodology to a simple tri-trophic microcosm prey-predator system (Hiltunen et al. 2013). The aim is to establish that the methodology developed is applicable in a simple ecological context. Overall, our method recovers ecological interactions that are consistent with the biology of the system (Arndt 1993; Hiltunen et al. 2013). Main interactions are conserved across the three replicated runs available for this system. Weaker interactions, between the intermediate predator and the prey, were not consistent. This chapter shows that ecological interactions may be inconsistent, even in systems that are virtually true replicates. Our study confirms that great care should be in order when generalising dynamics and processes across systems that appear repeatable (Lawton 1999). It also demonstrates the suitability of NODE to

infer dynamical interactions between biological variables.

In the final chapter, we use the method developed in the first chapter to provide quantitative evidence on eco-evolutionary feedbacks in the Darwin's finch system on Daphne Major island. We find evidence for indirect feedback effects between the finch population, beak morphology, and resource levels. We further find differences in feedback structure between the two closely related finch species on the island, and between the two morphological traits of each species. This suggests that we should expect a great diversity in feedback effects across species and systems (De Meester et al. 2019). This also confirms the importance of indirect feedback effects in driving rapid evolutionary responses (Hendry 2019). The following sections discuss the novelty and significance of these findings.

1.1 NODEs for ecological and evolutionary time series analysis

In chapter 1, we described how NODEs could be used to study eco-evolutionary dynamics from time series data (Bonnaffé, Sheldon, and Coulson 2021). We presented the mathematical requirements for implementing NODEs and explained how the coupling between the variables in the system could be recovered from the ANNs. We provided an example of NODE implementation by analysing the Hare-Lynx time series (Odum and Barrett 1972).

The main interest with using NODEs to study the interplay between ecological and evolutionary change lies in the capacity of ANNs to learn non-parametrically the processes that drive change. This is particularly useful when the processes at play are too complex to be modelled mathemati-

cally, or simply unknown (Jost and Ellner 2000; Wood 2001; Ellner, Seifu, and Smith 2002; Wu, Fukuhara, and Takeda 2005; Bonnaffé, Sheldon, and Coulson 2021). NODEs allow us to recover the shape of these processes, which can be used to obtain derived quantities, such as equilibrium points, or test different parametric models (e.g. Jost and Ellner 2000). However, from this strength also stems its main limitation, which is that NODEs do not directly recover mechanisms. NODEs should hence be viewed as a guide, or complement, to parametric models, rather than an alternative. Parametric models remain useful to test and compare different hypotheses. For instance, Jost and Ellner used a non-parametric function to learn the functional response of the prey to predator density. Once the shape of the functional response was identified, they compared it to different parametric constructions, such as Holling type I and II (Jost and Ellner 2000).

The second key contribution of the first chapter is the connection of the NODE framework to the Geber method (Hairston et al. 2005). We show how analysing NODE systems with the Geber method allows for the recovery of the dynamical coupling between variables. From an eco-evolutionary dynamics standpoint, this provides a non-parametric implementation of the Geber method, which is an invaluable counterpart to parametric implementations, in previous and future studies (e.g. Hairston et al. 2005; Ezard, Côté, and Pelletier 2009; Ellner, Geber, and Hairston 2011; Becks et al. 2012; Van Velzen and Gaedke 2017; Pigeon et al. 2017; Benthem et al. 2017). The correct estimation of feedback effects through the Geber method is contingent on a correct mathematical specification of the drivers of the dynamics, which may otherwise bias the inference. Our implementation reduces the chance of mis-representing the processes, and thereby feedback

effects, by finding the process shape that best describes the dynamics in the time series. From an Artificial Intelligence (AI) standpoint, the connection with the Geber method provides a way to make NODEs more interpretable. In AI, NODEs are primarily used for predictive modelling, or as a continuous alternative to residual neural networks (Chen et al. 2019). There were also several attempts to improve the interpretability of NODEs (Massaroli et al. 2020; Hu et al. 2020). For instance, Hu and colleagues used a polynomial basis for the ANNs in the NODE system to infer the effects between the variables (Hu et al. 2020). Our work goes further by allowing for the computation of the actual contribution of a variable to the dynamics of another, rather than simply looking at direct effects.

Perhaps the most beneficial and yet underexploited outcome of NODEs highlighted by our work is that it provides novel ways of estimating key dynamical properties. For instance, in this thesis, we showed how NODEs can be used to infer non-parametrically the Jacobian matrix, and find equilibrium points, simply by observing the dynamics of the system. This can be done by fitting the NODE system to the time series and then by differentiating the per-capita dynamics with respect to each variable in the system, or in the case of the equilibrium, by solving the NODEs (Bonnaffé, Sheldon, and Coulson 2021). We are not aware of another method that allows for the estimation of equilibrium points non-parametrically. The possibilities are limitless as NODEs could be used to infer other critical quantities such as the determinant, Hessian, which can be used to study further indirect effects between variables. This would provide a fascinating non-parametric way of studying press perturbations in natural communities (e.g. Montoya et al. 2009).

This also sets our work apart from the one other study that used ANNs embedded in an ODE skeleton to study ecological dynamics. Wu and colleagues used ANNs to approximate the functional response of a prey and a predator to population densities (Wu, Fukuhara, and Takeda 2005). This study was invaluable to provide a first example of application of NODEs, though they were not labelled as such in the study. Our work extends their framework by showing how the application of the Geber method to the NODE system could reveal dynamical coupling between the variables.

While NODEs in themselves are a novel addition to the field of ecology and evolution, they have been preceded by closely related non-parametric methods to study dynamical systems, called partially specified models (Jost and Ellner 2000; Wood 2001; Ellner, Seifu, and Smith 2002; Pasquali and Soresina 2018). These studies have in common the use of splines to learn biological processes non-parametrically from observations of the dynamics of the system. For instance, Pasquali used splines to learn non-parametrically the relationship between temperature and mortality in different development stage of the grape berry moth (Pasquali and Soresina 2018). The main difference between this approach and the NODE approach lies in the use of splines instead of ANNs. It should be noted that our NODE approach could be connected to that framework by choosing cubic splines as basis function in the single layer perceptron used in the first chapter (Bonnaffé, Sheldon, and Coulson 2021). NODEs can hence be viewed as a generalisation of the framework initially introduced by Wood.

1.2 Rotifer and identifiability of dynamics

In the second chapter, we apply NODEs to analyse ecological dynamics in three replicated runs of a three-species prey-predator microcosm (Hiltunen et al. 2013). The aim of this chapter was to establish the suitability of NODEs to study real biological dynamics in a slightly more complex system than the hare-lynx system. The system consisted of algae (prey), flagellates (intermediate predator), and rotifers (top predator). We considered three replicated runs of the system, all of which displayed similar prey-predator oscillations (Hiltunen et al. 2013). The NODE model was designed to approximate the per-capita growth rate of each species as a function of algae, flagellate, and rotifer density. We then compute the effect and contribution of each species to the growth rate of the other, and thereby the structure of the ecological network of interaction. We further compared these effects across the three replicated runs.

Overall, we found a dominant negative effect of the rotifer on the algae and flagellate, and a positive effect of the flagellate on the rotifer, across all replicates. This was consistent with previous work on this system, which established that rotifers exert strong top-down control on both populations (Arndt 1993; Hiltunen et al. 2013). This reinforces the idea that NODEs are suitable for gaining insights into the dynamics of real systems (Bonnaffé, Sheldon, and Coulson 2021).

Interestingly, we found that weaker effects were highly inconsistent in time and across replicates. The effect of the algae on the two predators, and the effect of the flagellate on the algae, varied from one replicate to the next. This was not accounted for by stochasticity in the variation of the population size because the deterministic non-parametric NODE approximation of growth rates

explained well the per-capita growth rates of the populations in the time series. Our results hence suggest that the variation in dynamics across the replicates may more readily stem from variation in initial conditions, probably in the genetic structure of the population (Becks et al. 2010; De Meester et al. 2019).

In this system the algae is prone to evolve an anti-predation behaviour, by forming clumps of cells, which reduces the efficiency of predation by flagellates and rotifers (Yoshida et al. 2003; Becks et al. 2012). What is surprising is that the authors that worked on the present system tried to lower genetic diversity in the algae as best as they could to reduce the chance of evolution altering the ecological dynamics of the system (Hiltunen et al. 2013). They may have thereby locked the different populations of the replicates into different areas of the phenotypic space, and thereby producing slightly different dynamical regimes (Becks et al. 2010).

More generally, these findings point at the problem of generalisation of dynamics across systems (Lawton 1999). The dynamics of the replicates may appear similar at first glance, but our NODE analysis reveals that they may in fact be underlined by slightly different networks of ecological interactions. This suggests a high level of context-dependence in ecological processes, even in virtually identical systems displaying seemingly identical dynamics.

It raises the question as to how often we may trust our findings to be generalisable. For instance, the evolution of guppy fish in Trinidad shows high levels of repeatability (Reznick 2016). Changes in population density and mean phenotype are comparable in streams that are completely disconnected. It remains an open question whether mechanisms that underlie these dynamics, namely

the architecture of eco-evolutionary feedback effects, display the same level of repeatability. Work on microcosms showed that while the outcome of evolution may be similar, it may be underlined by different mechanistic pathways for effects (Becks et al. 2012). This work, in addition to our study, and others (Brunner et al. 2019; Hendry 2019), suggest a poor degree of repeatability of mechanisms. More efforts should go towards quantifying context-dependency in effects (Brunner et al. 2019; Hendry 2019).

1.3 Interpolation technique to facilitate NODE fitting

In the second chapter, we also developed an alternative method for fitting NODEs, which relied on interpolating the time series. The time series are interpolated with sinusoid-based single layer perceptrons (SLPs). These provide approximations of the derivative of the variables in the system with respect to time, and thereby of the dynamics. The NODE system can then be fitted by finding the parameter vector that satisfies each NODE, given the interpolated variable states and temporal derivatives.

This implementation bypasses the need for solving the NODE system at every evaluation of the posterior distribution. It further provides analytically tractable gradients of the posterior with respect to each parameter in the NODEs. These two additions tremendously increase the speed of the fitting. In our previous chapter, we found that fitting the two-variable NODE system to the hare-lynx time series was taking over a minute. In this chapter, the interpolation-based fitting of the three-variable NODE system to the algae-flagellate-rotifer time series takes about half a sec-

ond. This speed is key to make it more feasible to quantify the reliability of fitting of the NODEs. NODEs are notoriously hard to fit (Chen et al. 2019), so that, in the context of the NODE literature, our approach provides a computationally efficient technique to fit these models. Our study could hence greatly facilitate the use of NODEs, which may be instrumental in making biologists adopt them.

The idea of interpolating the dataset to solve an ODE or a PDE system has been previously proposed in computational physics (e.g. Aarts and Van Der Veer 2001; Berg and Nyström 2019), and Biology (e.g. Ellner, Seifu, and Smith 2002; Wu, Fukuhara, and Takeda 2005). This idea has been used in three different ways. The initial technique proposed by Aarts and colleagues consists in fixing the parameters of the equations, and then training an ANN to produce likely trajectories for the variables of the system (Aarts and Van Der Veer 2001). The opposite approach consists in interpolating the data with ANN functions of time, then assessing the likelihood of different parametric equations given the interpolated time series. This is the approach used by Ellner and Berg (Ellner, Seifu, and Smith 2002; Berg and Nyström 2019). Berg used neural networks to interpolate temperature profiles in Sweden over a large geographic area and used the interpolated data to find suitable parametric PDE to describe the spatial distribution of temperatures. Ellner and colleagues developed a method called gradient matching where they used splines to approximate the time series of a prey and its predator. Then they would fit different parametric ODEs to the interpolated time series and temporal gradient of the prey to establish the most likely functional response to predator density. Wu and colleagues developed a hybrid approach, where the interpolated ANNs are fitted

to the time series, and the parametric equations are fitted to the interpolations, all at the same time. In this way the interpolation would also be trained to be consistent to the parametric equation. In all cases, the main benefit of the interpolation is that it circumvents the need for simulating the system and hence facilitates fitting.

Our approach is more akin to the technique used by Ellner (Jost and Ellner 2000; Ellner, Seifu, and Smith 2002), in the sense that the interpolation is performed before fitting the equations, rather than simultaneously. However, it builds upon and extends the work in two ways. We consider non-parametric equations, by fitting ANNs to the interpolation. We further embed the fitting approach in a Bayesian framework which provides a more reliable assessment of the error around the predictions of the NODEs.

1.4 Eco-evolutionary feedbacks in Darwin's Finches

In the final chapter, we used NODEs to infer eco-evolutionary feedbacks in Darwin's finches on Daphne Major island (Grant and Grant 1993). We inferred the drivers of change in seed supplies, population density of *G. fortis* and *G. scandens*, and population mean beak size and shape. To do that we modelled the dynamics of these variables as a NODE of the environmental, ecological, and evolutionary state of the system. For instance, changes in beak size in *G. fortis* were defined as a function of rainfall, small and large seeds, population density, mean beak size and shape. We fit the NODE system to the time series of each variable following the method developed in chapter 2 and 3. We then revealed the inter-dependencies between all variables.

We found that the eco-evolutionary feedback structure varied substantially between the two finch species. Feedbacks in *G. fortis* involved a negative effect of population density on the dynamics of the small seed supplies, which in turn had a positive effect on beak shape, and a negative effect on beak size. The feedback loop was closed by an effect of both traits, positive for beak size and negative for beak shape, on the population growth rate. These results are consistent with previous studies in this system. Carvajal and colleagues demonstrated a strong negative impact of the finch population on seed density (Carvajal-Endara et al. 2020). The Grants established that the radical switch from large to small seeds caused by the el Nino event selected strongly for smaller and more pointed beaks (Grant and Grant 1993). They further found highly inconsistent yet substantial contributions of beak morphology to the fitness of individuals from different cohorts (Grant and Grant 2000). Hairston and colleagues in their pioneering study revealed that beak size improved substantially the population growth rate throughout the time series (Hairston et al. 2005). However, they were unable to identify an effect of beak shape, probably in line with the low statistical power allowed by the short time series. We also found support for a shorter direct feedback loop between population density and phenotypic change in *G. fortis*. The Grants were suspecting a non-negligible, yet small, contribution of population density to the dynamics of the phenotype (Grant and Grant 2006). In this study we found that this effect was actually quite strong. Our results hence confirm some of the existing knowledge regarding the evolutionary response of the *G. fortis* population on the island, and extends our understanding of the feedback effects at play by demonstrating an indirect impact of seed predation on the evolution of *G. fortis*, and a direct feedback between population dynamics and phenotypic change.

In contrast, we did not find evidence for a coupling between phenotypic change and population dynamics in *G. scandens*. In the *G. scandens* population, phenotypic change is coupled with changes in medium seed supplies. Higher medium seed supplies tended to favour more pointed beaks, and in turn more pointed beaks tended to have a negative impact on medium seed supplies. In subsequent work, Peter and Rosemary Grant also found limited fitness consequences of changes in beak morphology in *G. scandens* (Grant and Grant 2000). They hypothesised that the unclear relationship between fitness and beak morphology in *G. scandens* may be due to contextual changes in the environment of the finch, and in particular in rainfall levels. This was later confirmed by Beausoleil and colleagues, who showed that the shape of the fitness landscape for beak morphology changed every year based on rainfall levels (Beausoleil et al. 2019). The difference in feedback structure between the two species is further consistent with the ecology of *G. scandens*, which is a specialist of medium seeds, contrary to *G. fortis*, which is more of a generalist (Grant and Grant 1993). *G. scandens* mainly relies on medium seeds, which are less strongly depleted following the el Nino event (Grant and Grant 1993). It is hence possible that the continued access to its main food source has dampened the evolutionary response of *G. scandens*, thereby leading to smaller impacts on demography. No study to our knowledge had investigated eco-evolutionary feedbacks at play in *G. scandens*, as most of the work focussed on the *G. fortis* population. Our work hence provides an unprecedented comparison of feedbacks between *G. fortis* and *G. scandens*.

Overall, finding such differences in the dynamics of two closely related species, sharing the same environment, suggests a high level of idiosyncrasy in feedback architecture. Our results hence

confirm the view that eco-evolutionary feedbacks may be highly context-dependent, and that small changes in the environment, ecology, or evolutionary state of the system may lead to radically different feedback structures (Brunner et al. 2019; Hendry 2019). An interesting question would then be to understand which contexts, namely which combinations of environmental, ecological, and evolutionary states, give rise to specific feedback architectures. For instance, in which context is evolution more readily resource-dependent, rather than density-dependent. And in which context is the demography more strongly affected by evolution than by environmental change. We would need more studies similar to this one across a wide range of systems to identify contextual factors that may lead to similar feedback structures.

Apart from this striking difference there were some elements of feedbacks conserved across the two species. First, the amount of rainfall on the island was a substantial driver of change in most of the variables in the system. This confirms the dominating impact of the el Nino event had in driving the eco-evolutionary dynamics of the finch populations (Grant and Grant 1993; Hairston et al. 2005). The second similarity lies in the importance of resources for the evolutionary dynamics in this system, given that the eco-evolutionary feedbacks at play in *G. fortis* and *G. scandens* both involved seed supplies. Our results hence further support the view that eco-evolutionary feedbacks involving resource predation and environmental variables may be ubiquitous (Brunner et al. 2019; Hendry 2019), as suggested in recent studies in guppies (Simon et al. 2017). Finally, although environmental effects were overall stronger than effects of resources and population density, phenotypic variables could in some cases exceed these effects. Beak morphology and population

density contributed to the same level as rainfall to the population growth rate in the *G. fortis* population. In *G. scandens*, changes in beak pointedness contributed more to the dynamics of medium seed supplies than rainfall itself. Our results hence confirm that the contribution of evolution to ecological dynamics can be as important and rapid as environmental change (Hairston et al. 2005; Ezard, Côté, and Pelletier 2009; Schoener 2011; Becks et al. 2012). This constitutes vital evidence as the relative importance of environmental, ecological, and evolutionary contributions is still an open question in many systems.

1.5 Limitations

There are several limitations to the NODE approach developed that we discuss here, starting with the applicability of the method for modelling biological systems. Perhaps the greatest strength, as well as limitation, of the method is that it is a non-parametric method. This means that it is suitable for identifying patterns and shapes of processes for which we do not have a suitable parametric construction. In particular, the NODE approach automatically handles interactions between variables, if they are required to explain the dynamics observed. This also sets it apart from spline-based dynamical models which do not efficiently deal with complex interactions between multiple variables (e.g. Jost and Ellner 2000; Wood 2001). However, NODEs do not provide the mechanism that underpins the patterns found, which requires further parametric investigations. In this sense, NODEs are powerful for beachheading theoretical investigations, but are not a substitute for parametric models. In addition to this aspect, it should be noted that we have applied NODEs to study eco-evolutionary feedback where they are known to be at play. The NODEs framework in

itself does not allow to establish the evolutionary nature of phenotypic change. This is a limitation shared by all model fitting techniques. To overcome this limitation, we would need more data documenting heritable genetic change in real systems, as well as model structures specifically designed to distinguish between evolutionary change and plasticity (e.g. Ellner, Geber, and Hairston 2011). Finally, the modelling framework considered here is fully deterministic. Coupled with Bayesian inference, it allows to partition variation in the data into observation and process error (Calder et al. 2003). In this way it does not directly quantify the importance of stochasticity in driving changes in the state variables of the system. An interesting prospect for development would be to incorporate explicitly stochasticity in the model, with stochastic differential equations (Mao, Yuan, and Zou 2005; Jia and Benson 2019).

The second general type of limitation to the NODE framework developed here lies in the inference process. Artificial neural networks are notoriously hard to train, so are ODE models. NODEs, by combining these two components are particularly challenging to fit (Chen et al. 2019). The posterior distribution of the parameters is not mathematically tractable because solving ODEs requires numerical approximations. That, in addition to the large number of parameters required by the neural networks, makes it hard to navigate the parameter space in search of local maxima. There are more sophisticated techniques to compute gradients of the model (e.g. Rackauckas et al. 2019), but these are computationally intensive, and hard to implement. This further causes several problems for the inference of NODE parameters. We often cannot identify a single model, due to a highly heterogenous posterior distribution, which reduces model identifiability. This requires a more in-

tensive search of the parameter space, by running the fitting procedure multiple times, compared to simpler statistical frameworks. This also requires the use of regularisation techniques, which increases model identifiability by constraining parameters with arbitrary prior distributions (e.g. Cawley and Talbot 2007). These techniques have the tendency, however, to bias the estimation of quantities approximated by the NODEs because they artificially reduce the variance and mean of the network parameters, especially at higher levels of constraint. In order to account for this, one needs to assess the robustness of the results to different regularisation levels. Ultimately, larger datasets, for instance, longer time series and multiple system states, can help dealing with model identifiability, and reduce the need for regularisation.

Finally, in this thesis, we have developed two techniques for fitting NODEs. The first method consists in simulating numerically the NODE system over the time steps covering the time series data (Chen et al. 2019). Then, the model parameters are adjusted to improve the fit of the simulated trajectory to the value of the state observed in the time series. The second method, called gradient-matching, consists in interpolating the time series of state variables, and then fit the NODEs to the interpolations (Ellner, Seifu, and Smith 2002). In this way, there is no need for simulating the model, which provides analytical expressions for the gradients. These two methods have their respective strengths and limitations. The first method allows to obtain results that are dynamically consistent, which means that the processes inferred (e.g. species interactions) produce the trajectories of the state variables (Wu, Fukuhara, and Takeda 2005). This makes the method suitable for further dynamical analysis of the model, for instance, for finding equilibrium points, or identifying

attractors. The downside is that the simulation step is computationally intensive and prevents the use of analytical gradient-descent methods. In contrast, the second method is much faster, and allows for a faster acquisition of approximate posterior distributions, and higher model identifiability thanks to a more efficient search of the parameter space. But the approach is not dynamically consistent given that each time series are interpolated and fitted independently. The benefit of this, however, is that the results found for each time series are not contingent on obtaining a successful fit of the NODEs to the other time series, whereas this is a requirement for the first method. This means that the second method might identify effects between variables that may be missed by the first method, where all changes have to be consistent with one another.

1.6 Prospects

We see several ways in which NODEs could be used to generate further insights into eco-evolutionary dynamics. The most obvious prospect would be to apply NODEs across a variety of systems for which we have ecological and evolutionary time series. A chosen candidate would be the guppy system in Trinidad (Reznick et al. 2019). The guppy system features time series for the environmental variables (stream discharge, sunlight exposure), ecological variables (population density, biomass of invertebrates, algae), and evolutionary variables (body length at maturity). These time series are available for four replicates located in different streams in Trinidad. Analysing this dataset with NODEs would provide another quantitative example of feedback structure, and the unique opportunity to observe the repeatability of eco-evolutionary feedbacks across independent systems by comparing results across these natural replicates.

In spite of their non-parametric nature, NODEs could also be potentially useful in driving theoretical investigations. The first way would be to test the consistency of different parametric ODEs with the non-parametric approximations provided by the NODEs. For instance, we could propose a parametric equation for the per-capita growth rate of the *G. fortis* population, and infer the value of the parameters by fitting the ODE to the NODE approximation, similarly to the work of Jost and Ellner (Jost and Ellner 2000). In this way, we translate the NODE system into a parametric ODE system, and thereby find likely mechanisms. The second way is to incorporate mechanisms directly in the NODE system, similarly to what Wu and colleagues propose (Wu, Fukuhara, and Takeda 2005). That is, the NODEs could incorporate functions that describe dynamical processes that we would like to enforce in the system. More concretely, this amounts to using ANNs more strategically to infer specific biological functions, by embedding them in a parametric equation. For instance, we could use the framework developed by Ellner, which consists in using the price equation to model phenotypic dynamics (Ellner, Geber, and Hairston 2011). In this construction the ODE describing phenotype dynamics contains two sources of change, change through evolution, modelled by the product of the additive genetic variance of the trait and the selection gradient, and a second term, capturing plastic changes in the phenotype throughout the life of an individual. We could define the per-capita growth rate of the population, and thereby the selection gradient as an ANN function. In this way, we could use NODEs to a slightly more mechanistic end, by inferring additive genetic variance, selection, and plasticity from time series of phenotypes. This would provide a valuable connection to the mountain of theoretical models merging quantitative genetics and ODE systems (e.g. Cooke et al. 1990; Day and Gandon 2007; Queller 2017; Lion

2018; Patel, Cortez, and Schreiber 2018).

One final and exciting prospect would be to extend NODEs to neural partial differential equations (NPDEs) and neural integral projection models (NIPMs). The benefit of this would be to include structure of natural systems in the models, either spatial structure, or phenotypic structure. For instance, one could use NPDEs to study eco-evolutionary dynamics in continuous space, such as the evolution of seed dispersal in wind-dispersing plants. In such a system, local dynamics are determined by the local conditions, namely the local state of phenotypic, demographic, and environmental variables (e.g. wind speed), but also potentially by conditions at all other locations. In this case, it may be more suitable to rely on PDEs instead of ODEs to model the spatio-temporal dynamics of the population. In a standard PDE we would need to add two terms, one describing the outgoing dispersal of individuals towards other sites, and ingoing dispersal from all other sites to the local site. These terms would be given by the convolution of a dispersal kernel on the spatial distribution of the phenotype and environmental variables. We often lack suitable equations for these kernels (Dalziel, Morales, and Fryxell 2008). We could hence use an NPDE instead, by defining the dispersal kernels as ANN functions of location, phenotype, and environmental conditions, which would turn the NPDE istelf into a convolutional neural network (CNN). We may hence learn the shape of the dispersal kernels from time series of the spatial dynamics of populations (e.g. statellite images), with no prior knowledge about the underlying mechanisms. The technique developed in this thesis to fit NODEs by interpolating time series data could easily be extended to create multivariate interpolations and potentially facilitate the inference of NPDEs.

This would benefit a colossal body of work on spatial eco-evolutionary dynamics (e.g. Hanski 2011; Hanski and Mononen 2011; Hanski et al. 2017). NIPMs would stand as the discrete time counterparts of NPDEs. They could be useful to model the drivers of change of phenotype and breeding value distributions in species with discrete (e.g. yearly) breeding cycles (e.g. Childs, Sheldon, and Rees 2016). Similarly to the NPDEs, we could use ANNs to learn the survival, growth, reproduction, heritability kernels embedded in the integrals. The use of the interpolation technique developed in this thesis would allow to fit the IPM directly to the time series, instead of parametrising the kernels beforehand. As far as we are aware, no study has combined IPMs with ANNs, which would be a useful addition given the prosperous and strong rooting of IPMs in the ecological literature (e.g. Childs, Sheldon, and Rees 2016; Coulson et al. 2011; Simmonds and Coulson 2015; Gamelon et al. 2019).

1.7 Conclusion

The aim of this thesis was to provide quantitative evidence for eco-evolutionary feedbacks at play in iconic natural systems. In the first chapter, we designed a novel method, combining ordinary differential equations, artificial neural networks, and Bayesian inference, to infer unknown dynamical processes non-parametrically from time series data. We connected the framework with the Geber method, which allows us to quantify the strength of the coupling between the key variables in the system. Given the non-parametric nature of the model, no assumptions are required regarding the nature of the processes, which allows for a more objective quantification of effects than with parametric models where prior mechanistic knowledge is lacking. This represents a

substantial improvement for the identification of the drivers of change in natural systems in an eco-evolutionary context, given the complexity of the processes involved, and the lack of consensual specific methodology.

In the second chapter, we applied the method developed in the first chapter to identify the drivers of the dynamics in a three-species prey-predator sytem involving a prey, an intermediate predator, and a top predator. We found that the main ecological interactions, between the top predator and the prey, were consistent across the replicates of the system, contrary to weaker interactions, involving the intermediate predator. This work demonstrates the suitability and power of NODEs for resolving ecological interactions between different species, as well as showing the inconsistent nature of dynamical processes, which varied substantially across replicates.

In the third chapter, we apply the method to quantifying the eco-evolutionary feedbacks at play in the Darwin's finches system on Daphne Major island. We found substantial differences in the feedback structure between the medium ground finch and cactus finch. Feedbacks in the medium ground finch involved a strong coupling between population dynamics and phenotypic change, whereas in the cactus finch, changes in phenotype were more readily coupled with changes in seed supplies. Our work hence provides precious quantitative and comparative evidence for eco-evolutionary feedbacks at play in a real system, showing the importance of indirect effects mediated by changes in resource levels and population density, as well as the potential idiosyncratic nature of effects. Overall, this thesis points at the huge potential for NODEs to push empirical and theoretical investigations further in all fields dealing with the dynamics of biological systems.

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