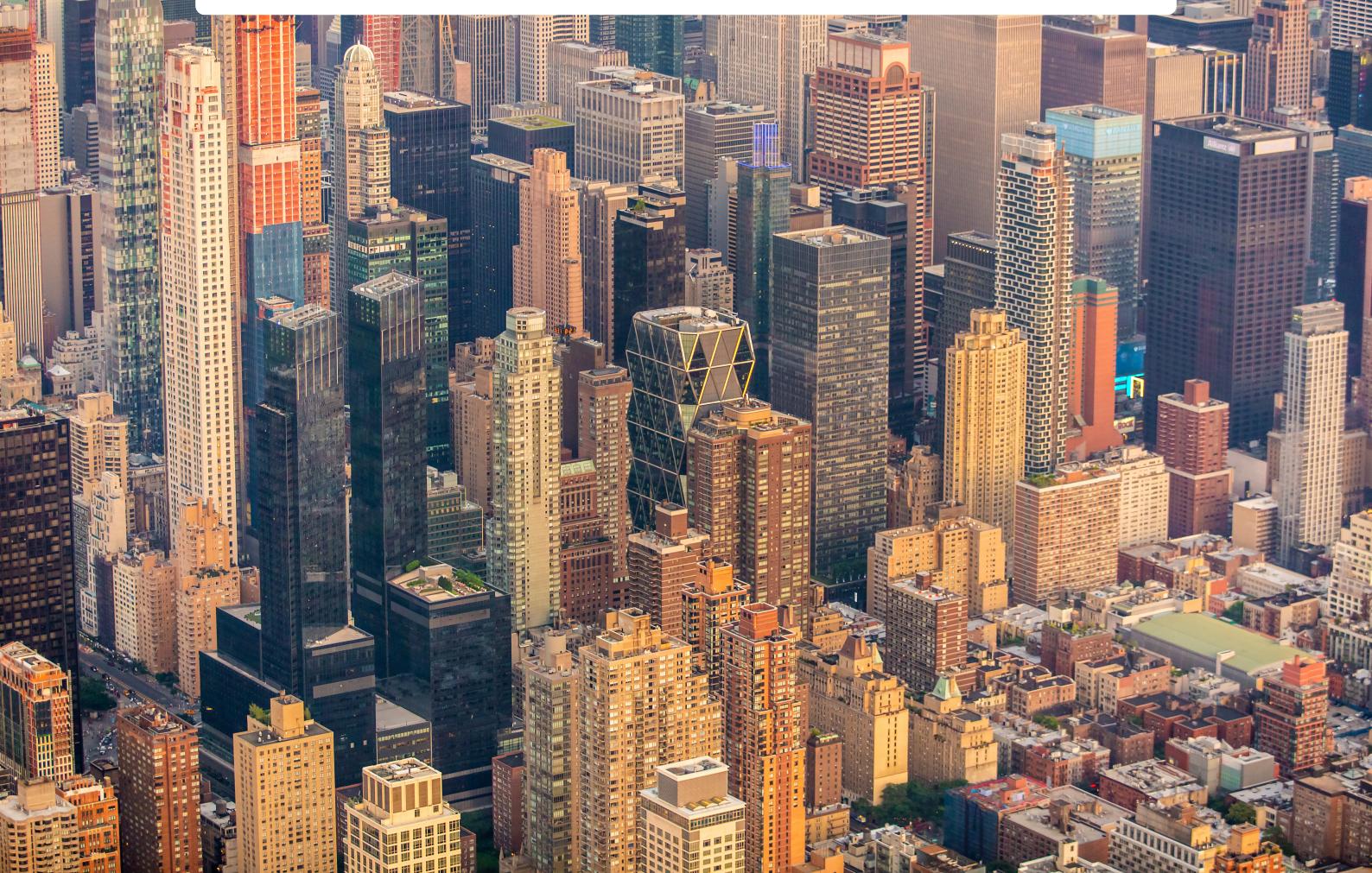


Forward and inverse modelling of eco-evolutionary dynamics

in biological and economic systems

Victor BOUSSANGE



Victor Boussange

Forward and inverse modelling of eco-evolutionary dynamics in biological and economic systems

September 17, 2022

Cover picture: Top: forest in Sorapiss, Dolomites, Italy. Bottom: New York City, USA. @ Luca
Bravo / PhotoSpirit

The document format is based on the *Clean Thesis* style developed by Ricardo Langner.

Acknowledgement

What a journey! Four years ago, I have decided to embark on a ship to live a big adventure. Worrigly lacking sailing experience, I still envisioned a voyage in unknown seas, at the crossroads between biology, economics, and applied mathematics. I wanted to experience storms and dangers because, as Alfred Maufray said, "À vaincre sans périls, on triomphe sans joie". But honestly, I was not expecting so much! Here are some words that cannot express all the gratitude I have towards these wonderful people that have accompanied me all along this journey, and without whom I could not have made it safe back home.

I thank my supervisor, Loïc Pellissier, who allowed this expedition by providing the necessary ingredients: a boat and a map. Loïc, thank you so much for allowing me the freedom to draw the exact route, while kindly indicating me the north when I was lost. I thank Arnulf Jentzen for guiding me through the strange sea of applied mathematics, besides my lack of mathematical rigor. Arnulf, thank you for your forgiveness and patience, I have come a long way! I thank Didier Sornette for welcoming some crazy ideas with enthusiasm, and give it scientific substance with his experience and knowledge. I thank Thomas Poulet for his mentorship through ought the voyage. Thomas, you taught me the most important rudiment required to sail! I thank Heike Lischke for her help in crucial times. I thank all my friends and colleagues from the Landscape Ecology group. Special thanks to Giulia Donati and Camille Pitteloud for introducing me to Zürich, and to the world of research. The times when you were in the lab were the most beautiful and funny moments of the voyage. Special thanks to Charles de Novaes and Benjamin Flück, who respectively introduced me to Julia and helped me with amazing efficiency when I was about to throw my computer in the bin (which I did, but only once). Special thanks to Conor Waldock, Marc Grünig and Alex Skeels for their help and kindness. You guys always had the right advice at the right time!

I also thank all my wonderful friends, who allowed me to gain my motivation back and continue the journey. Special thanks to Théo Lafitte, Matthieu Demolin, Yoann Roncajolo, Diego Parlange and Luc Thiebaut for sharing wine, waves and fun. Special thanks to Simon Ducroz, Valentin Mathieu, Mathieu Duthoit, Baptiste Le Maire, Guillaume Chabert and Alexandre Martineau for sharing moments of sheer beauty and happiness in the high alpine. Special thanks to my riding buddies Morgan Guening and Daniel Grogg for introducing me to enduro mountainbiking,

and for sharing sheer moments of joy and adrenaline. Life in Zürich would have been very different without you guys! Special thanks to my climbing buddies Anita Herger and Jonas von Wartburg, for sheer moments of bliss and philosophy, and Tuesday night German and climbing sessions.

A massive thank-you to my family for their support. Sabine, Clémentine and Marc, thank you so much for always having been here with me. And last but not least, I thank Flora for making every second of this life worth remembering. I'll never be as good of a sailor as you are, but we'll become two captains very soon.

Contents

1 Discussion	1
1.1 Contributions	1
1.1.1 Advancing our fundamental understanding of eco-evolutionary processes in biological and economic systems	1
1.1.2 Leveraging forward and inverse modelling with ML	5
1.2 Limitations	8
1.2.1 Forward modelling	8
1.2.2 Inverse modelling	10
1.3 Perspectives	11
1.4 Concluding remarks	14
2 CV	15
List of Figures	25

Discussion

”

*To be but one with all living things, to return, by
a radiant self-forgetfulness, to the All of Nature.*

— Friedrich Hölderlin (1770-1843)

1.1 Contributions

Understanding biological and economic systems involves the underpinning of the elemental processes underlying the systems' macroscopic features, and establishing the associated mechanisms (Levin, 2002, ??). Following this approach, my work aimed at advancing our understanding of how ecological and evolutionary processes, and their interplay, shape the dynamics of biological and economic systems. In particular, this thesis contributed to

- (i) a fundamental understanding of the role of eco-evolutionary processes in shaping the dynamics of biological populations structured in complex landscapes ??,
- (ii) the quantification of the effect of mechanisms associated with eco-evolutionary processes in economic systems ??,
- (iii) methodological advances in the forward and inverse modelling of eco-evolutionary dynamics ??????.

In the following, I discuss the chapters of my thesis collectively within the broader context of our current understanding of the dynamics of biological and economic systems, and the accompanying modelling paradigm.

1.1.1 Advancing our fundamental understanding of eco-evolutionary processes in biological and economic systems

Linking eco-evolutionary processes to patterns of differentiation

Spatial patterns of biodiversity result from the processes of selection, mutation and dispersal, that act upon individual organisms ([hamilton2021population](#)). In finite size populations, mutations result in "drift" ([Slatkin1987a](#)), causing stochastic

variations in the allelic proportions and phenotypes of biological populations. In geographically structured population, drift results in patterns of neutral differentiation (**Slatkin1987a**), where isolated populations are characterised by differentiated allelic proportions and phenotypes. Dispersal tends to reduce neutral differentiation (**Slatkin1987a**), and this effect is modulated by landscape connectivity (Wright, 1943; McRae, 2006; McRae and Beier, 2007) through the mechanism of "isolation by limited dispersal" (Orsini et al., 2013). By increasing the dispersal ability of organisms, landscape connectivity decreases neutral differentiation (Lande, 1991). When landscapes present heterogeneous habitats, natural selection can supplement the effect of genetic drift and increase the sole effect of stochasticity on differentiation (**fisher1958genetical**). Under this scenario, local environment conditions select individuals with traits that provide them higher fitness (**Gaither2018**). At the population level, this results in populations adapting to their local environment, a mechanism coined "local adaptation" (Kawecki and Ebert, 2004) and resulting in patterns of "adaptive differentiation". Adaptive differentiation is hindered by dispersal, which prevents local adaptation by bringing maladapted individuals, that destabilise the evolution of traits towards the optimal (Meszéna et al., 1997; Débarre et al., 2013; Mirrahimi and Gandon, 2020). While adaptive differentiation concerns traits under selection, it indirectly affects the differentiation of neutral traits, that are co-evolving with traits under selection through linkages (Billiard et al., 2015; Lepers et al., 2021). This results in turn to the mechanism of "isolation by adaptation", where habitat heterogeneity, rather than landscape connectivity, increases neutral differentiation (**nosil2008**). Simple mechanisms resulting in neutral and adaptive differentiation are identified, but how they are modulated by eco-evolutionary feedbacks and landscape complexity is unclear.

In ??, I demonstrate a novel mechanism, involving the process of intra-specific competition, that considerably affects neutral differentiation. Through the creation of unbalanced migration fluxes which increases the intensity of competition in highly connected populations, heterogeneity in connectivity reduces gene flow and reinforces neutral differentiation. I also investigate how the mechanism of local adaptation in complex landscapes, where habitats are arranged in a realistic fashion. I show that the complexity of habitat spatial distribution can be reduced to a measure of habitat spatial auto-correlation, coined the "habitat assortativity". Landscapes characterised by a high habitat assortativity systematically support populations that are locally better adapted than in landscape with low assortativity, resulting in higher adaptive differentiation. Specifically, I provide an analytical condition for local adaptation that sheds light on how it relates to dispersal intensity, selection strength, habitat heterogeneity, and habitat assortativity.

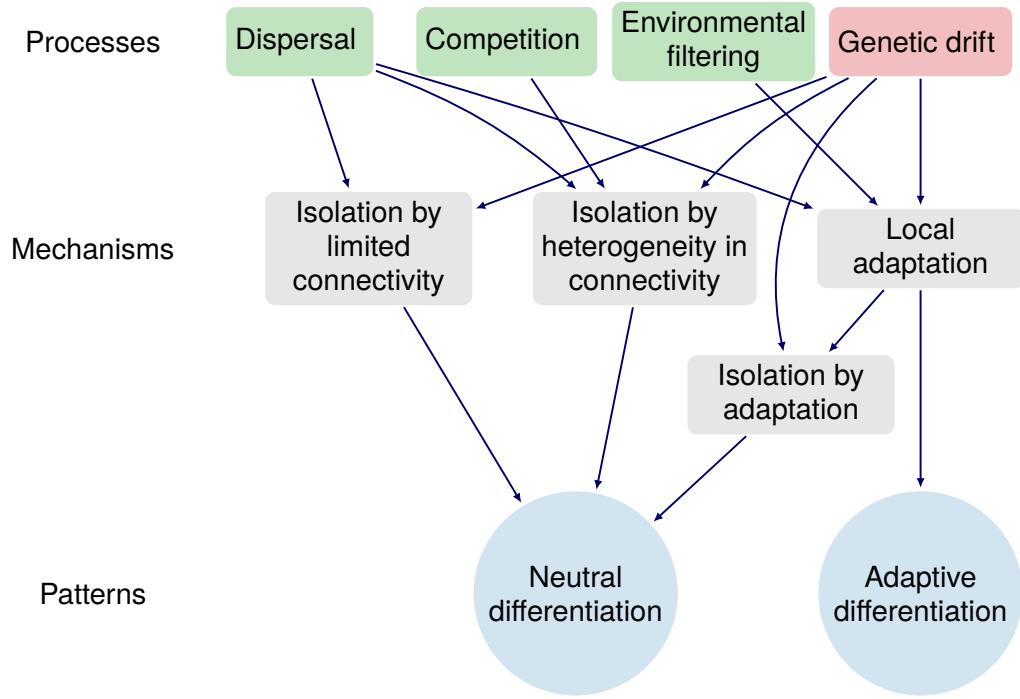


Fig. 1.1: Summary of the causal pathways involved in neutral and adaptive differentiation, disentangled in ?? . Ecological processes are displayed in green boxes, evolutionary processes are displayed in red boxes.

Because habitat assortativity affects local adaptation, it must also affect neutral differentiation through the mechanism of isolation by adaptation. Closing the loop, I demonstrate that habitat assortativity affects population differentiation through two antagonistic effects. By favoring local adaptation, it promotes isolation by adaptation, therefore increasing neutral differentiation. In parallel, it also favors gene flow within clusters of similar environmental conditions, decreasing isolation by limited dispersal. This results in habitat assortativity decreasing neutral differentiation for low dispersal intensity, and increasing neutral differentiation for high dispersal intensity. This complex feedback is essential to understand population differentiation in complex landscapes.

I provide a summary of the processes and resulting mechanisms shaping neutral and adaptive differentiation in Fig. 1.1. Overall, ?? links processes to patterns, establishing an extensive map of causal pathways involved in the phenotypic differentiation of populations.

Linking economic patterns to eco-evolutionary processes

?? provides a novel understanding of the role of eco-evolutionary processes in economic systems. Neoclassical economics and evolutionary economics seek to explain

economic change with formal modelling, focusing on the relationships between economic variables such as output, employment and productivity (Boschma and Frenken, 2005). In particular, evolutionary economics is concerned with explaining economic change by endogenous forces, such as interactions between firms and economic activities, and evolutionary processes acting upon them (Metcalfe2006; Hodgson, 2019). In opposition to this approach, complexity economics (Hidalgo, 2021) seeks to predict variations in national income by using fine-grained data of economic activity outputs and dimensionality reduction techniques (Mitchell, n.d.), without making assumptions on the underlying processes (Hidalgo). While a current concern in evolutionary economics is to obtain an agreement between the mechanisms proposed and empirical observations (XXX), complexity economics seeks to understand the causal processes underlying the success of the dimensionality reduction technique (XXX).

By being agnostic to economic variables yet providing a causal link with the most probable processes underlying economic development, ?? bridges evolutionary economics and economic complexity. Our approach relies on the simple observation that the dynamics of economic activities contains signatures from the many complex processes that underpin them. These signatures consist in peculiar temporal variations and couplings that can be conveniently modelled by biologically inspired population dynamic models, which use are additionally justified by deep analogies between economic activities and biological populations. Analogously to biological populations that are characterised by genes, economic activities are characterised by organizational routines (NelsonWinter), which experience evolutionary processes and define how they engage in ecological processes (NelsonWinter). As a result, and similarly to the size of biological populations, the capital growth of economic activites is determined by the ensemble of organizational routines that characterise them (Boschma and Frenken, 2005). Similarly to approaches used in ecology and evolution (Skeels), inverse modelling approaches can then be used to disentangle, from their signatures (Skeels) left on the dynamics of economic activities, the role of the eco-evolutionary processes acting upon them.

Specifically, ?? explores the effect of eco-evolutionary processes, proposed in the evolutionary economics and geography economics literature, on the dynamics of economic activities at the national scale. In particular, ?? seeks to test whether the dynamics of economic activities can be explained by different types of interdependencies, including positive (XXX) and negative interactions (XXX), spatial transfers (XXX), and economic transformations (XXX). Using population dynamic models capturing the different interdependencies, ?? provides empirical evidence that economic activities engage in positive interactions, and benefit from spatial transfers of knowledge and routines. Positive interactions may arise from a variety of processes

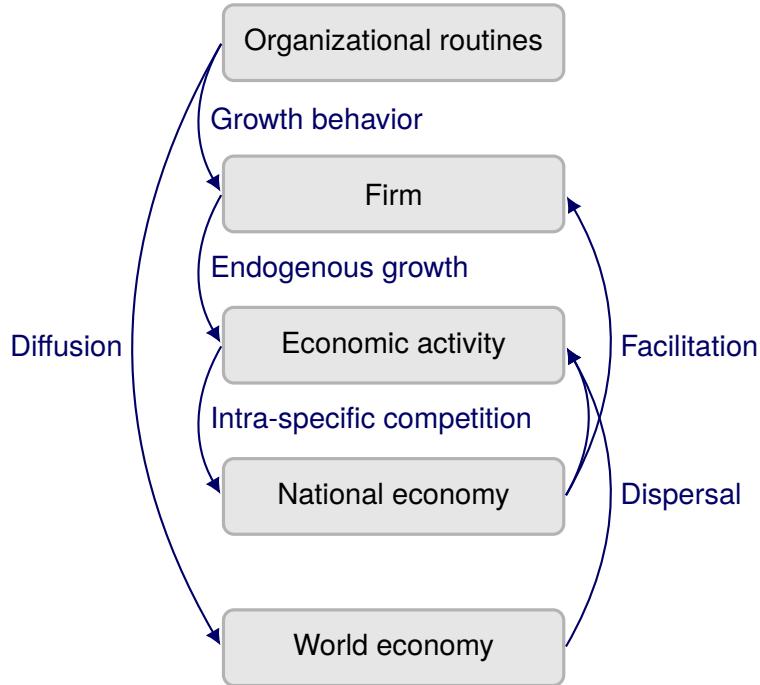


Fig. 1.2: Summary of the eco-evolutionary processes evidenced in ??, and how they affect the different organizational levels in economic systems.

proposed in the evolutionary economic literature, such as supply chains (Ozman, 2009; Saavedra et al., 2009) and knowledge spillovers (Menon, 2015). Its support implies that diversity promotes economic development (**Hidalgo2018**), as economic activities promote each other. The support for spatial transfers implies that, besides international patent laws (XXX), transfers of knowledge and organisational routines have a considerable effect on economic activities. Nevertheless, discrepancies in the strength-of-evidence obtained for spatial transfers across countries highlight that some countries are overall more akin to spatial transfers than others, which may be explained by differences in cognitive, organizational, social, institutional or geographic proximities across countries (XXX). I provide a summary of the mechanisms evidenced in economic systems in Fig. 1.2. Overall, ?? bridges approaches in economics and biology to understand the mechanisms shaping the endogenous dynamics of economic systems.

1.1.2 Leveraging forward and inverse modelling with ML

Advances in the modelling of realistic spatial and phenotypic structures

???? provide new tools to better understand mechanisms resulting from ecological and evolutionary processes, and their interplay, in the context of realistic population

structures and phenotypic distributions. Evolutionary dynamics have been traditionally studied in the context of regular population structures (Lieberman et al., 2005). For instance, Slatkin, 1973; Slatkin, 1978; Kirkpatrick and Barton, 1997; Polechová and Barton, 2015; Polechová, 2018; AndradeRestrepo et al., 2019; Doeblei and Dieckmann, 2003; Meszéna et al., 1997; Yeaman and Otto, 2011; Débarre et al., 2013; Mirrahimi and Gandon, 2020 consider regular spatial structures to investigate differentiation in biological populations, missing the effect of spatial complexity on the underlying mechanisms. Biological habitats differ in their connectivity (XXX), and economic entities are structured through complex networks (XXX). Lieberman et al., 2005 and subsequent studies of "evolutionary dynamics on graphs" (XXX) show that this complexity affects the interplay between selection and drift. However, evolutionary dynamics on graphs does not consider eco-evolutionary feedbacks (Govaert2019a). Thus far, models that include frequency dependence together with realistic, complex population structures were missing.

While a vast majority of the work on eco-evolutionary feedbacks has focused on the evolution of scalar phenotypes (Doebeli2011), in most organisms, many phenotypic properties combine in complicated ways to determine ecological processes (Doebeli2014). For instance, Doebeli2011 shows that the consideration of multiple traits is likely to generate more diversity than expected with one dimensional models. Trade-offs in traits is also an essential feature shaping the evolutionary dynamics of biological populations, with consequences on the dynamics of e.g. cancer cell evolution (XXX) and plankton dynamics (XXX). While there is overall a genuine need to better understand evolutionary dynamics in high dimensional spaces, the simulation of high dimensional models is tremendously difficult, since the numerical cost of traditional methods grows exponentially in the number of dimensions of the phenotypic space.

?? develops a generic modelling framework to capture the effect of eco-evolutionary processes on biological populations structured in complex landscapes, and ?? provides tools to efficiently simulate the resulting high-dimensional models. The IBM presented in ?? involves the combination of graphs and highly dimensional phenotypic spaces, together with eco-evolutionary feedbacks, to model population structures. The modelling framework presented can readily be generalised, and the code associated to the numerical experiments in ?? include a Julia library, **Evoid.jl**, that implements a more general version of the model. As such, the modelling framework presented in ?? may be used to investigate other questions involving complex population structures and the co-evolution of characteristics. Reproducing the discrete and stochastic nature of ecological and evolutionary processes (Champagnat et al., 2006), simulations of the IBM may not provide a general understanding of system investigated (XXX), and cannot be scaled to simulate large systems involving

millions of individuals (XXX). Nevertheless, the IBM proposed in ?? is mathematically tractable under simplifying assumptions, and can be efficiently simulated with a deterministic PDE approximation. Tractability allows to obtain analytical insights on how structural properties affect macroscopic population under simplifying assumptions (??). The PDE approximation, combined with the numerical methods presented in ??, further allow efficient simulations. I have implemented the numerical methods for simulating high dimensional models in the Julia library **HighDimPDE.jl** (**HighDimPDE**), a registered Julia package belonging to the SciML organisation (XXX). The user interface respects standards from the SciML organisation, meaning that Julia users can easily adopt it. The package aims at hosting many more solver algorithms that break down the curse of dimensionality, and is currently receiving contributions from developers to implement the DeepBSDE scheme (Han et al., 2018).

The combination of analytical insights and numerical simulations can help to elucidate the links between microscopic processes and macroscopic properties (**Levin**). ???? provide novel analytical and numerical tools to better understand how complex spatio-evolutionary structures affect the interplay between eco-evolutionary processes and generate macroscopic patterns.

Advances in inference methods for the investigation of eco-evolutionary processes

???? develop and test a novel inverse modelling method that allows to infer highly nonlinear dynamical processes from observation data, opening up new venues to advance our understanding and prediction of the dynamics of biological and economic systems. The most developed inference methods in current use for inverse modelling are Bayesian inference methods with Markov Chain Monte Carlo (XXX) and variational methods (XXX). Bayesian inference methods require a large number of forward model integrations (Schneider et al., 2017), and are highly affected by the number of model parameters (**Csillary2010**). Variational methods require the model sensitivity to its parameters (XXX) and are prone to converge to local minima, especially with complex models (XXX). Those central issues likely explain the very poor number of studies that have used inverse modelling to further our knowledge on eco-evolutionary dynamics (XXX).

? presents a novel inference framework that can efficiently recover the most probable parameter values of eco-evolutionary models, given temporal data. The framework is based on a variational method, but resolves its main shortcomings by including key ingredients in the recipe, including automatic differentiation (Rackauckas et al., 2020), state-of-the-art optimizers (Kingma and Ba, 2014), and a

learning strategy based on a mini-batch method. The use of automatic differentiation simply eliminates the effort required to obtain the model sensitivity to its parameters, and the state-of-the-art optimizers, together with the mini-batch method, ensure the efficiency and reliability of the method in handling highly nonlinear models. ?? is part of an ongoing effort to blend ML and traditional models to gain scientific understanding and extrapolability (XXX). In physical systems such as ocean and atmospheric systems (XXX), invariant laws are known, and ML is mostly used to improve model forecast skill. In contrast, models of biological and economic systems are yet to be formulated, methods such as the the ML framework presented in ?? can greatly contribute to gain scientific knowledge. By contrasting competing hypotheses embedded in alternative models, ???? provide concrete examples, both with synthetic and empirical data, that the ML framework can successfully elucidate eco-evolutionary mechanistic pathways. The proposed method is also relevant for improving the forecast of predictive eco-evolutionary model Urban et al., 2016, and integrates the practical constraints of datasets including short time series with partial, noisy, shallow and independent observations (Dornelas et al., 2018).

The ML framework is implemented in the multi-purpose Julia package **MiniBatchInference.jl** (**MiniBatchInference**), readily available to the scientific community. **MiniBatchInference.jl** is built around the celebrated differential equation solver **DifferentialEquations.jl** and the deep learning library **Flux.jl**. As such, the use of **MiniBatchInference.jl** requires very limited efforts to any user familiar with those libraries.

Overall, the method proposed in ?? successfully blends ML methods with mechanistic ecosystem models to improve our gain scientific knowledge from observation data. Concrete case examples in ???? show that it enables the testing of eco-evolutionary theories against data, advancing our understanding and the improvement of current mechanistic models, with the potential to provide better forecasts of ecosystems states (Urban et al., 2016).

1.2 Limitations

1.2.1 Forward modelling

Alternatives to the methods presented in ???? may be more appropriate for the forward modelling of eco-evolutionary dynamics. While IBMs are interesting tools to investigate stochastic drift in finite size populations, the Gillespie algorithm (Gillespie, 1976) used to simulate the IBM in ?? is computationally intensive, and requires to compute the fitness of all individuals at each time step, which depends on the characteristics of all the other individuals. The resulting computational

complexity grows polynomially with the number of individuals ($\mathcal{O}(N^2)$). While it is an interesting tool to investigate stochastic drift in finite size populations, it cannot be used to model large populations. On the other hand, PDEs can provide deterministic approximations of IBMs (Champagnat et al., 2006), while demanding less computational power. The methods presented in ?? can approximate PDEs in high dimensions (up to 10 traits, which seems more than enough in practice (XXX)), but still suffer from a number of issues that may prevent their practical use. In particular, the MLP method can only provide the population density for one single trait value, and as such, cannot characterise the total population density with a reasonable computational complexity. On the other hand, the ML based approximation method can provide the full population density, but involves the training of many neural networks, one at each time step. This is worrying, since the training of a neural network is numerically costly, and that long simulation times may be required by practitioners. An other problem with the numerical methods proposed in ?? is that they involve the tuning of meta parameters, inluding the choice of a kernel for the integration of the nonlocal term. This choice is critical for the success of the approximation, but how to determine it is not clear . Together, the methods proposed in ?? may require further development to be used in practice by practitioners. Yet irrespective of the numerical method used, solving PDEs inevitably requires a considerable computational effort, because PDEs track the evolution of the full phenotypic density of populations. Nevertheless, only the first three moments of the population density are usually of interest to investigate eco-evolutionary dynamics (population size, trait mean and trait variance, see XXX). Instead of seeking to numerically approximate the full phenotypic density, moment closure approximation methods (Wickman2021; Lion2022; Nordbotten et al., 2020) may be, so far, more appropriate tools. Those approaches consist in approximating the population density with a gaussian distribution. This, in turn, allows to transform the PDE problem into a sytem of coupled differential equations involving the time evolution of the population size (1 variable for a single species population), the mean trait value in each dimension of the trait space (d variables), and the variance-covariance matrix of the trait density (d^2 variables). As such, the computational cost of this method scales only polynomially with the number of dimension ($\mathcal{O}(d^2)$), while providing the exact information required to investigate eco-evolutionary dynamics in high dimensional spaces. It is worth noting that instead of neural networks, gaussian functions could easily be used with the ML-based approximation method to simulate PDEs. Equivalent to the assumption taken in the moment closure methods presented in Wickman2021; Lion2022; Nordbotten et al., 2020, we expect that this approach would greatly improve the computational efficiency of the ML-based approximation method in simulating eco-evolutionary models, while solving the problem of the

choice of a kernel for the integration of the nonlocal term. Using Gaussian functions may considerably lower the number of iterations required in the training process, while reducing the computational cost, as they involve less parameters ($d(d + 1) + 1$) than neural networks (xx in ??).

1.2.2 Inverse modelling

The inverse modelling framework proposed in ?? and used in ?? also present shortcomings, which may favor the use of other methods to infer eco-evolutionary processes from data. First, the mini-batching learning strategy requires the choice of a minibatch size to ensure the convergence to the maximum likelihood estimate. This choice is arbitrary, but may affect the model selection process. Reducing the batch size implies that the model is fitted on the short term dynamics of the data, but because the model is likely to only characterise some of the features of the data, the resulting support could differ, were the model rather fitted to long term dynamics. Theoretical developments will be required to better understand the assumptions behind the choice of the mini-batch size, which may provide guidance to the choice of this meta parameter. Second, the proposed method may fail to find the maximum likelihood estimate of complex models, since the associated likelihood landscape is harder to navigate than simpler ones. This may lead to a bias in the model selection process towards simpler models. Third, the information criterion-based model selection procedure used in ???? is uniquely based on a trade-off between goodness-of-fit and number of parameters of the model, which may not be satisfactory to characterise the complexity of dynamical models. For instance, XXX shows that the logistic map, which consists of only two parameters, can be fitted to any pattern. Other criterion, involving the complexity of the dynamical behavior of the model (such as, e.g., its Lyapunov exponent), could as such be developed. Fourth, the ML framework developed in ?? requires a differentiable model, a strong prerequisite that may not be met by stochastic models (XXX). Fifth, the ML framework provides a single point estimate of the posterior distribution, which is subsequently used for model selection. Yet the models' posterior distributions may be multimodal, where the alternative modes carry valuable information to consider in the model selection process (Daniels2015). In this case, fully Bayesian method may be required to characterise the full posterior distribution. Alternatively, Skeels2022 employs a more flexible approach for model selection, which does not require differentiability. The method consists in aggregating model simulation outputs into summary statistics, which are used to train classifier algorithms in recognizing the generating model. The classifier algorithms, such as random forests and neural networks, are further used on summary statistics obtained from the empirical data, recovering the most

likely models and associated hypotheses. This approach is similar to Approximation Bayesian Computation methods **Csillary2010**, and requires summary statistics that can correctly discriminate between models. This is a strong requirement to grant the success of the model selection procedure, but it has the major advantage of clarifying why the model is more likely.

Overall, the methods presented in **????** solve major problems arising in the forward and inverse modelling of eco-evolutionary dynamics, but suffer from shortcomings. These limitations may direct practitioners to alternative methods, but also invite to further developments.

1.3 Perspectives

Development opportunities in inverse modelling

The mini-batch method developed in **??** and the ML-based approximation method developed in **??** offer unique development opportunities to leverage inverse modelling. The mini-batch method is relevant beyond the ML framework presented in **??**, and could be used within a fully Bayesian framework (**XXX**), where the full posterior distribution of the model is estimated. While Bayesian inference with MCMC chains methods may not be appropriate for eco-evolutionary models (see **??**), automatic differentiation variational inference (ADVI, **XXX**) offers an appealing alternative. With ADVI, the posterior distribution is approximated by a gaussian distribution (**XXX**), significantly reducing the number of model integration (Gosh et al., 2021). Improving the ML framework presented in **??**, ADVI could capture multimodality in the model posterior distribution (by approximating the multimodal distribution with a gaussian distribution with large variance). This, in turn, could improve the model selection procedure (**??**), and provide uncertainties measures to the value of the parameters inferred. Providing uncertainty estimates while ensuring computational efficiency, Bayesian Learning via Stochastic Gradient Langevin Dynamics (**Welling2011BayesianIV**) could also be implemented in the ML framework. This method builds upon recent advances in Bayesian Deep Learning (**Wilson2020**) and interprets the iterative gradient-based optimization procedure as a Markov chain with an equilibrium distribution over the posterior distribution of the model parameters. It therefore comes with the scalability of variational methods and the interpretability of Bayesian methods, and can provide good estimates of uncertainty errors for complex models.

The ML-based approximation method for high dimensional PDEs, presented in **??**, could be used for inverse modelling. In **??**, the parameters of the PDE model are assumed fixed, but could be set as free parameters, analogously to the parameters

of the neural networks used for approximating the solution. The loss function in ?? would then take the PDE model parameters as additional arguments, and include an additional term, involving the distance between the PDE model solution and the data. This term, analogous to ?? in ??, would constrain the PDE parameters, similarly to the training of physics informed neural networks (Raissi et al., 2019; Yazdani et al., 2020). In contrast to Raissi et al., 2019; Yazdani et al., 2020, a major advantage of this approach it to efficiently perform inverse modelling with high-dimensional dynamical models. Because Julia is a programming language with pervasive AD, this development would require little effort with the Julia library **HighDimPDE.jl**. Together, the ML methods developed in ???? offer unique development opportunities to bring more robustness and efficiency to inverse modelling methods, providing uncertainty estimation and the possibility to handle high dimensional models.

Confronting eco-evolutionary model on spatial graphs and empirical data

The confrontation of the predictions from ?? with empirical data, and the use of inference methods with the proposed eco-evolutionary model on spatial graphs, could advance our understanding of eco-evolutionary dynamics in empirical systems. ?? proposed topology metrics that should correlate with standard population differentiation metrics (Q_{ST} metrics). Because real landscapes can be projected on spatial graphs ((XXX)and ??), the topology metrics, together with empirical data on population differentiation (e.g., **Fluerin**), could be used to verify our predictions. Discrepancies may indicate that other important processes may be involved in empirical patterns. On the other hand, a validation of our predictions could help to predict population differentiation at a global scale. These predictions could, in turn, be linked to patterns of species richness, in order to underpin how population genetics may lead to speciation over time (XXX). In the same direction, the use of the eco-evolutionary model on spatial graphs, together with paleo-climatic data (**HagenXXX**) and inference methods, could help addressing fundamental questions on the processes involved in current biodiversity patterns. ?? succinctly tests whether our predictions hold for a more general setting involving trait-based competition. Trait-based competition may be ubiquitous in biological systems (XXX), and similarly to the process of environmental filtering (XXX), can lead to diversification. An important question on the research agenda is to underpin how competition may mediate environmental filtering and promote and hamper diversification over time. This fundamental question could be addressed by embedding the competing hypotheses in alternative models, which support could be tested against data. Along shorter time scales, the eco-evolutionary model on spatial graph could be calibrated on empirical data of species distribution (XXX)with the inference method proposed

in ??, and combined with climate scenarios (XXX) to better predict how biological populations will adapt to climate change (Norberg et al., 2012; Urban et al., 2016). Together, the model developed in ?? and the resulting predictions, together with the ML framework presented in ??, could bring insights on the actual mechanisms involved in empirical systems, and help to predict their responses to climate change.

Econobiology, a new venue to understand economic systems, and design more appropriate governance

The current understanding of key processes and patterns in biological systems may provide insights into organization principles in economic systems, and provide guidance for economic policies. The biologically inspired eco-evolutionary model presented in ?? was successful in characterizing the dynamics of economic activities. ?? therefore evidences deep connections between processes acting upon economic and biological systems. On top of encouraging the characterization of these processes at a finer level, this calls for investigating parallels in the dynamics and organizational principles between biological and economic systems. There may be connections between nutrient cycles in ecosystems (**Veldhuis2018**) and capital cycles in economic systems (**King1993**), where ecological compartments and financial intermediaries develop to improve the efficiency of nutrient flows and capital allocations (Odum, 1969). **Veldhuis2018**; **King1993** show that this efficiency sustains productivity and growth, but the developmental process may fail, where ecosystems stay in a state of lower maturity (**Margalef1963**) or technological lock-in (**Hidalgo2009**). What are the links between the evolution of nutrient and capital cycles, and the fundamental processes acting upon lower organization levels? Future directions should seek to understand at a finer level the processes evidenced in ??, and understand how they may result in organizational principles at the economy level. **Veldhuis2018** provides a synthesis of our understanding of how ecosystem organization emerges through self-reinforcing mechanisms, promoted by ecological and evolutionary processes acting upon producers, consumers, and decomposers. This synthesis provides an interesting roadmap, and analogous self-reinforcing mechanisms could play important roles in determining fluxes of capital in economic systems. The quest for finding common organizational principles may help us distinguishing important differences between economic systems. Since biological systems have undergone evolution for a much longer time than economic systems, they may be more effective and resilient than economic systems. These differences may inspire economic policies. Altogether, biology may eventually help us understanding organizational principles in economic systems, and provide guidance for improving economic regulations.

1.4 Concluding remarks

It is, more than ever before, urgent to better understand and forecast the dynamics of life on Earth. While we know that the global temperature on Earth will rise by 2 to 4 degrees in 2100, predictions on ecosystem states are much more uncertain. Yet obtaining more realistic ecosystem forecasts is critical to help designing adequate management of ecosystem services. Blending scientific knowledge, formalised in mathematical model, with machine learning, provides unique opportunities to quickly improve our understanding of ecosystem dynamics and provide forecasts. Machine learning is part of the astonishing technological progress experienced by humankind in the last centuries. This progress has led us to think that we are rational beings, that have crafted singular socio-economic to create wealth. Yet it may well be that socio-economic systems are analogous to, but less efficient and resilient than, biological systems. Leaving aside our navel gazing, we could surely get insights from organizational principles in ecosystems, that have survived major environmental crisis for more than 3.5 billion years. To conclude, let us cite Hölderlin: "*To be but one with all living things, to return, by a radiant self-forgetfulness, to the All of Nature*".

Personal Information

Residence	Zürich, Switzerland
E-mail	bvictor@ethz.ch
Website	vboussange.github.io
Github	github.com/vboussange
Age	Born 1995 (age 27)
Citizenship	France citizen

Personal skills

Languages	English (fluent) French (native) Spanish (B2) German (B1)
Programming languages	Julia Python C++ Java Matlab R Bash VBA
Sports	Ski mountaineering Alpinism Rock climbing Enduro mountainbiking Surfing
Alpine CV	[vboussange.github.io/pages/alpine_cv/]

Education

- 10.2022 **Ph.D in Environmental Sciences**, Swiss Federal Institute for Forest, Snow and Landscape (WSL | Swiss Federal Institute of Technology Zurich, ETH), Switzerland
Forward and inverse modelling of eco-evolutionary processes in biological and economic systems. Under the guidance of Prof. Dr. Loïc Pellissier.
- 06.2017 **Full year academic exchange**, University of New South Wales (UNSW Sydney), Australia
- 06.2017 **Master thesis in theoretical geomechanics**, UNSW Sydney | CSIRO, Australia
Numerical continuation and bifurcation analysis for unconventional geomechanics. Under the guidance of Dr. Thomas Poulet.
- 08.2018 **M.S. in Energy and Environmental Engineering**, Institut National Des Sciences Appliquées de Lyon (INSA Lyon), France
Three-year undergraduate engineering course in Energy and Environmental Systems, focused on Advanced Energy Systems and Efficiency.
- 08.2018 **B.S. in Mathematics and Physics**, Institut National Des Sciences Appliquées de Lyon (INSA Lyon), France
Ranking : 21/650 students.

Professional appointments

- 08.2018 **R&D intern**, Compagnie National du Rhône (CNR), France
03.2018 Development of an Energy Management System based on various optimisation techniques for optimal production of renewable resources. Applications to EU sponsored projects: **Jupiter1000** (power-to-gas), **Move in pure** (vehicle-to-grid), **Marie-Galante island** (micro-grid)

Publications

Peer-reviewed

1. **Boussange, V.** & Pellissier, L., *Eco-evolutionary model on spatial graphs reveals how habitat structure affects phenotypic differentiation*. *Commun Biol* 5, 668 (2022). [[bioRxiv](#)]

Preprints

1. **Boussange, V.**, Vilimelis-Aceituno, P., Pellissier, L., *Mini-batching ecological data to improve ecosystem models with machine learning* [[bioRxiv](#)] (2022), 46 pages. In review.
2. **Boussange, V.**, Becker, S., Jentzen, A., Kuckuck, B., Pellissier, L., *Deep learning approximations for non-local nonlinear PDEs with Neumann boundary conditions*. [[arXiv](#)] (2022), 59 pages. Revision requested from Partial Differential Equations and Applications.

Proceedings

1. Poulet, T., Alevizos, S., Veveakis, M., **Boussange, V.**, Regenauer-Lieb, K., *Episodic mineralising fluid injection through chemical shear zones*, ASEG Extended Abstracts (2018), 5 pages.

In preparation

1. **Boussange, V.**, Sornette, D., Lischke, H., Pellissier, L., *Analogous forces to ecological interactions, dispersal and mutations shape the dynamics of economic activities*.

Talks

- 07.2022 **Speaker**, HIGHDIMPDE.JL: A Julia package for solving high-dimensional PDEs, JuliaCon2022, online. [youtube.com/watch?v=4sXqGhhknT4](https://www.youtube.com/watch?v=4sXqGhhknT4)
- 06.2022 **Speaker**, Interpretable machine learning for forecasting dynamical processes in ecosystems, World Biodiversity Forum, Davos, Switzerland.
- 06.2022 **Invited speaker**, Investigating empirical patterns of biodiversity with mechanistic eco-evolutionary models, Seminar at the Theoretical Ecology and Evolution group, Universität Bern.
- 11.2021 **Invited speaker**, Numerical approximations of solutions of highly dimensional, non-local nonlinear PDEs, StAMBio seminar, St Andrews, UK.
- 10.2021 **Speaker**, Graph topology and habitat assortativity drive phenotypic differentiation in an eco-evolutionary model, Conference on Complex Systems, Lyon, France.
- 10.2021 **Speaker**, Using graph-based metrics to assess the effect of landscape topography on diversification, ECBC, Amsterdam, Netherlands.
- 09.2021 **Speaker**, Solving non-local nonlinear Partial Differential Equations in high dimensions with HighDimPDE.jl, International Conference on Computational Methods in Systems Biology, Bordeaux, France.
- 04.2021 **Speaker**, Responses of neutral and adaptive diversity to complex geographic population structure, Mathematical Population Dynamics, Ecology and Evolution, CIRM Marseille, France.

Softwares

- 2022 **MiniBatchInference.jl** Julia
github.com/vboussange/MiniBatchInference.jl
A Julia package for maximum likelihood estimation and model selection of strongly nonlinear dynamical models.
- 2021 **HighDimPDE.jl** Julia
github.com/vboussange/HighDimPDE.jl
A Julia package that breaks down the curse of dimensionality in solving non local, non linear PDEs.
- 2021 **EvoId.jl** Julia
2019 github.com/vboussange/EvoId.jl

Evolutionary individual based modelling, mathematically grounded.

- 2018 **OptiVPP** Python, GAMS
confidential
Energy Management System for Virtual Power Plants.

Open source software contributions

SciML
DiffEqFlux.jl
CUDA.jl
Flux.jl
LightGraphs.jl

Teaching and supervision

12.2020 **701-3001-00L Environmental Systems Data Science**, ETH Zürich, D-USYS,
09.2020 Switzerland

06.2020 **262-0100-00L Lab rotation**, ETH Zürich, D-BSSE, Switzerland
04.2020

12.2020 **Taste of research internship**, Polytech Nice-Sophia, France
09.2020

Reviews

- 2022 **Journal of Open Source Software**
2019 **Journal of Theoretical Biology**

Bibliography

- AndradeRestrepo, Martín, Nicolas Champagnat, and Régis Ferrière (2019). “Local adaptation, dispersal evolution, and the spatial ecoevolutionary dynamics of invasion”. In: *Ecology Letters* 22.5. Ed. by Vincent Calcagno, pp. 767–777 (cit. on p. 6).
- Billiard, Sylvain, Régis Ferrière, Sylvie Méléard, and Viet Chi Tran (2015). “Stochastic dynamics of adaptive trait and neutral marker driven by eco-evolutionary feedbacks”. In: *Journal of Mathematical Biology* 71.5, pp. 1211–1242. arXiv: 1310.6274 (cit. on p. 2).
- Boschma, Ron A and Koen Frenken (2005). “Why is economic geography not an evolutionary science? Towards an evolutionary economic geography”. In: (cit. on p. 4).
- Champagnat, Nicolas, Régis Ferrière, and Sylvie Méléard (2006). “Unifying evolutionary dynamics: From individual stochastic processes to macroscopic models”. In: *Theoretical Population Biology* 69.3, pp. 297–321 (cit. on pp. 6, 9).
- Débarre, F., O. Ronce, and S. Gandon (2013). “Quantifying the effects of migration and mutation on adaptation and demography in spatially heterogeneous environments”. In: *Journal of Evolutionary Biology* 26.6, pp. 1185–1202 (cit. on pp. 2, 6).
- Doebeli, Michael and Ulf Dieckmann (2003). “Speciation along environmental gradients”. In: *Nature* 421.6920, pp. 259–264 (cit. on p. 6).
- Dornelas, Maria, Laura H. Antão, Faye Moyes, et al. (2018). “BioTIME: A database of biodiversity time series for the Anthropocene”. In: *Global Ecology and Biogeography* 27.7, pp. 760–786 (cit. on p. 8).
- Gillespie, Daniel T. (1976). “A general method for numerically simulating the stochastic time evolution of coupled chemical reactions”. In: *Journal of Computational Physics* 22.4, pp. 403–434 (cit. on p. 8).
- Gosh, Sanmitra, Paul Birrell, and Daniela De Angelis (2021). “Variational inference for non-linear ordinary differential equations”. In: *Proceedings of The 24th International Conference on Artificial Intelligence and Statistics* 130.29, pp. 2719–2727 (cit. on p. 11).
- Han, Jiequn, Arnulf Jentzen, and Weinan E (2018). “Solving high-dimensional partial differential equations using deep learning”. In: *Proc. Natl. Acad. Sci. USA* 115.34, pp. 8505–8510 (cit. on p. 7).
- Hidalgo, César A. (2021). “Economic complexity theory and applications”. In: *Nature Reviews Physics* 3.2, pp. 92–113 (cit. on p. 4).
- Hodgson, Geoffrey M. (2019). *Evolutionary Economics*. Vol. 66. Cambridge University Press, pp. 37–39 (cit. on p. 4).
- Kawecki, Tadeusz J. and Dieter Ebert (2004). “Conceptual issues in local adaptation”. In: *Ecology Letters* 7.12, pp. 1225–1241 (cit. on p. 2).

- Kingma, Diederik P. and Jimmy Ba (2014). "Adam: A Method for Stochastic Optimization". In: *arXiv:1412.6980*, 15 pp. arXiv: 1412.6980 (cit. on p. 7).
- Kirkpatrick, Mark and N. H. Barton (1997). "Evolution of a Species' Range". In: *The American Naturalist* 150.1, pp. 1–23 (cit. on p. 6).
- Lande, R. (1991). "Isolation by distance in a quantitative trait". In: *Genetics* 128.2, pp. 443–452 (cit. on p. 2).
- Lepers, Clotilde, Sylvain Billiard, Matthieu Porte, Sylvie Méléard, and Viet Chi Tran (2021). "Inference with selection, varying population size, and evolving population structure: application of ABC to a forwardbackward coalescent process with interactions". In: *Heredity* 126.2, pp. 335–350. arXiv: 1910.10201 (cit. on p. 2).
- Levin, Simon A. (2002). "Complex adaptive systems: Exploring the known, the unknown and the unknowable". In: *Bulletin of the American Mathematical Society* 40.01, pp. 3–20 (cit. on p. 1).
- Lieberman, Erez, Christoph Hauert, and Martin A. Nowak (2005). "Evolutionary dynamics on graphs". In: *Nature* 433.7023, pp. 312–316 (cit. on p. 6).
- McRae, Brad H. (2006). "ISOLATION BY RESISTANCE". In: *Evolution* 60.8, p. 1551 (cit. on p. 2).
- McRae, Brad H. and Paul Beier (2007). "Circuit theory predicts gene flow in plant and animal populations". In: *Proceedings of the National Academy of Sciences* 104.50, pp. 19885–19890 (cit. on p. 2).
- Menon, Carlo (2015). "Spreading big ideas? The effect of top inventing companies on local inventors *". In: *Journal of Economic Geography* 15.4, pp. 743–768 (cit. on p. 5).
- Meszéna, Géza, István Czibula, and Stefan Geritz (1997). "Adaptive Dynamics in a 2-Patch Environment: A Toy Model for Allopatric and Parapatric Speciation". In: *Journal of Biological Systems* 05.02, pp. 265–284 (cit. on pp. 2, 6).
- Mirrahimi, Sepideh and Sylvain Gandon (2020). "Evolution of specialization in heterogeneous environments: equilibrium between selection, mutation and migration". In: *Genetics* 214.2, pp. 479–491 (cit. on pp. 2, 6).
- Mitchell, Melanie (n.d.). "Analogy-Making as a Complex Adaptive System". In: () (cit. on p. 4).
- Norberg, Jon, Mark C. Urban, Mark Vellend, Christopher A. Klausmeier, and Nicolas Loeuille (2012). "Eco-evolutionary responses of biodiversity to climate change". In: *Nature Climate Change* 2.10, pp. 747–751 (cit. on p. 13).
- Nordbotten, Jan Martin, Folmer Bokma, Jo Skeie Hermansen, and Nils Chr Stenseth (2020). "The dynamics of trait variance in multi-species communities". In: *R. Soc. Open Sci.* 7.8, Article No. 200321, 20 pp. (Cit. on p. 9).
- Odum, Eugene P. (1969). "The strategy of ecosystem development". In: *Science* 164.3877, pp. 262–270 (cit. on p. 13).

- Orsini, Luisa, Joost Vanoverbeke, Ine Swillen, Joachim Mergeay, and Luc De Meester (2013). “Drivers of population genetic differentiation in the wild: Isolation by dispersal limitation, isolation by adaptation and isolation by colonization”. In: *Molecular Ecology* 22.24, pp. 5983–5999 (cit. on p. 2).
- Ozman, M. (2009). “Inter-firm networks and innovation: a survey of literature”. In: *Economics of Innovation and New Technology* 18.1, pp. 39–67 (cit. on p. 5).
- Polechová, Jitka (2018). “Is the sky the limit? On the expansion threshold of a species’ range”. In: *PLoS Biology* 16.6, pp. 1–18 (cit. on p. 6).
- Polechová, Jitka and Nicholas H. Barton (2015). “Limits to adaptation along environmental gradients”. In: *Proceedings of the National Academy of Sciences of the United States of America* 112.20, pp. 6401–6406 (cit. on p. 6).
- Rackauckas, Christopher, Yingbo Ma, Julius Martensen, et al. (2020). “Universal Differential Equations for Scientific Machine Learning”. In: arXiv: 2001.04385 (cit. on p. 7).
- Raissi, M., P. Perdikaris, and G.E. Karniadakis (2019). “Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations”. In: *Journal of Computational Physics* 378, pp. 686–707 (cit. on p. 12).
- Saavedra, Serguei, Felix Reed-tsochas, and Brian Uzzi (2009). “A simple model of bipartite cooperation for ecological and organizational networks”. In: *Nature* 457.7228, pp. 436–466 (cit. on p. 5).
- Schneider, Tapiro, Shiwei Lan, Andrew Stuart, and João Teixeira (2017). “Earth System Modeling 2.0: A Blueprint for Models That Learn From Observations and Targeted HighResolution Simulations”. In: *Geophysical Research Letters* 44.24, pp. 12,396–12,417. arXiv: 1709.00037 (cit. on p. 7).
- Slatkin, Montgomery (1973). “GENE FLOW AND SELECTION IN A CLINE”. In: *Genetics* 75.4, pp. 733–756 (cit. on p. 6).
- (1978). “Spatial patterns in the distributions of polygenic characters”. In: *Journal of Theoretical Biology* 70.2, pp. 213–228 (cit. on p. 6).
- Urban, M. C., G. Bocedi, A. P. Hendry, et al. (2016). “Improving the forecast for biodiversity under climate change”. In: *Science* 353.6304 (cit. on pp. 8, 13).
- Wright, Sewal (1943). “Isolation By Distance”. In: *Genetics* (cit. on p. 2).
- Yazdani, Alireza, Lu Lu, Maziar Raissi, and George Em Karniadakis (2020). “Systems biology informed deep learning for inferring parameters and hidden dynamics”. In: *PLOS Computational Biology* 16.11. Ed. by Vassily Hatzimanikatis, e1007575 (cit. on p. 12).
- Yeaman, Sam and Sarah P. Otto (2011). “Establishment and maintenance of adaptive genetic divergence under migration, selection, and drift”. In: *Evolution* 65.7, pp. 2123–2129 (cit. on p. 6).

List of Figures

- | | | |
|-----|---|---|
| 1.1 | Summary of the causal pathways involved in neutral and adaptive differentiation, disentangled in ??. Ecological processes are displayed in green boxes, evolutionary processes are displayed in red boxes. | 3 |
| 1.2 | Summary of the eco-evolutionary processes evidenced in ??, and how they affect the different organizational levels in economic systems. . | 5 |

