The following individuals certify that they have read, and recommend to the Faculty of Graduate and Postdoctoral Studies for acceptance, the dissertation entitled:

**Evolution and maintenance of diversity in ecological communities**

submitted by **Ilan Naftali Rubin** in partial fulfillment of the requirements for the degree of **Doctor of Philosophy** in **Zoology**.

**Examinining Committee:**

Michael Doebeli, Professor, Zoology and Mathematics, UBC  
*Supervisor*

Laura Parfrey, Associate Professor, Zoology and Botany, UBC  
*Supervisory Committee Member*

Sarah Otto, Professor, Zoology, UBC  
*University Examiner*

Kermit Ritland, Emerita, Forest and Conservation Sciences, UBC  
*University Examiner*

**Additional Supervisory Committee Members:**

Christoph Hauert, Professor, Mathematics, UBC  
*Supervisory Committee Member*

Rosemary Redfield, Emerita, Zoology, UBC  
*Supervisory Committee Member*
Abstract

Understanding the mechanisms that generate and maintain diversity in ecological communities is perhaps the central question of ecological theory. Early theoretical contributions by Robert MacArthur formalized multi-species coexistence by considering how frequency dependent competition can naturally partition a continuous trait space into distinct niches. More recently, the adaptive dynamics framework has extended these ecological dynamics based on frequency dependent interactions to evolutionary timescales, creating a model capable of describing adaptive speciation and the emergence of diversity through natural selection. In this thesis I expand on these theories to help provide a greater understanding of the mechanisms that drive species coexistence and the maintenance of variation in ecological communities. In Chapter 2 I compare the diversity on ecological versus evolutionary timescales by comparing the diversity of randomly assembled communities to that of the ESS (evolutionary stable state, and the theoretical endpoint of evolution). I show that when randomly assembled, ecological communities can be saturated (having a diversity greater than the evolutionary stable state), yet saturation becomes prohibitively hard in higher dimensions. In Chapter 3 I show how Red Queen evolutionary dynamics can trap communities in low diversity metastable states. In Chapter 4 I combine perhaps the two most iconic theories of evolutionary diversity, the rugged fitness landscape and negative frequency-dependence, into one model. In doing so I show how on very rugged landscapes evolutionary dynamics mimic the local optimization and stochastic peak-shift dynamics predicted by rugged fitness landscape theory. However, the diversity each system can support is determined by the relative strength of frequency dependence and the shape of the global landscape, not the ruggedness. In Chapter 5 I consider the evolution of phenotypic heterogeneity, i.e., when genetically identical individuals have different phenotypes. I show that there is a race between diversification leading to a population of specialists and the evolution of heterogeneity, which leads to a division of labor.
Lay Summary

When Charles Darwin introduced the ideas of natural selection and survival of the fittest, he brilliantly explained how variation can be generated through natural, evolutionary mechanisms. However, it was not until much later that formal theory was able to explain the stable coexistence of many competitors. In this thesis I use mathematical models to help broaden our understanding of how diversity emerges and is maintained through natural selection. I investigate how the diversity of ecosystems changes between ecological and evolutionary timescales; show that the same ecosystem can support communities with vastly different numbers of species; compare two classical models of evolutionary dynamics: the rugged fitness landscape and niche-packing; and explore under what conditions evolution may select for diversification rather than a division of labor.
Preface

A version of Chapter 2 has been published as a preprint as: I. Rubin, Y. Ispolatov, and M. Doebeli (2022). Ecological diversity exceeds evolutionary diversity in model ecosystems. bioRxiv 2022.03.24.485441. and is under peer review for publication. I was responsible for initial conceptualization, model development, coding, analysis, interpretation of the results, and writing the manuscript; Y. Ispolatov for interpretation of results and manuscript editing; and M. Doebeli for initial conceptualization, interpretation of the results, and manuscript editing.

A version of Chapter 3 has been published as: I. N. Rubin, I. Ispolatov, and M. Doebeli (2021). Evolution to alternative levels of stable diversity leaves areas of niche space unexplored. PLOS Computational Biology 17(7), e1008650. I was responsible for conceptualization, model development, coding, analysis, interpretation of the results, and writing the manuscript; I. Ispolatov for coding, interpretation of results, and manuscript editing; and M. Doebeli for conceptualization, model development, supervision of the project, and manuscript editing.

A version of Chapter 4 has been published as a preprint as: I. N. Rubin, Y. Ispolatov, and M. Doebeli (2022). Adaptive diversification and niche packing on rugged fitness landscapes. bioRxiv 2022.05.15.492034. and is under peer review for publication. I was responsible for initial conceptualization, model development, coding, analysis, interpretation of the results, and writing the manuscript; Y. Ispolatov for interpretation of results and manuscript editing; and M. Doebeli for interpretation of the results and manuscript editing.

A version of Chapter 5 has been published as: I. N. Rubin and M. Doebeli. Rethinking the evolution of specialization: A model for the evolution of phenotypic heterogeneity (2017). Journal of Theoretical Biology 435, 248-264. I was responsible for initial conceptualization, model development, coding, analysis, interpretation of results, and writing the manuscript and M. Doebeli was responsible for interpretation of results, supervision of the project, and manuscript editing.
# Table of Contents

Abstract ........................................................................................................ iii

Lay Summary .................................................................................................. iv

Preface ........................................................................................................... v

Table of Contents .......................................................................................... vi

List of Tables ................................................................................................. x

List of Figures ............................................................................................... xi

Acknowledgements ......................................................................................... xiii

1 Introduction ................................................................................................. 1
  1.1 Thesis goals ............................................................................................. 3
  1.2 General modelling approach ................................................................. 3
    1.2.1 Note on stability ................................................................................ 4
    1.2.2 Remarks on the definition of species ............................................. 5
  1.3 Chapter 2 ................................................................................................. 5
  1.4 Chapter 3 ................................................................................................. 5
  1.5 Chapter 4 ................................................................................................. 6
  1.6 Chapter 5 ................................................................................................. 6

2 Ecological diversity exceeds evolutionary diversity in model ecosystems .... 8
  2.1 Introduction ............................................................................................. 8
  2.2 Methods .................................................................................................. 9
    2.2.1 Ecological Dynamics ....................................................................... 9
    2.2.2 Ecological simulations ..................................................................... 10
    2.2.3 Calculation of the ESS ................................................................... 11
  2.3 Results .................................................................................................... 11
    2.3.1 ESS and Evolutionary dynamics .................................................... 11
    2.3.2 ESS is the endpoint of evolution .................................................... 11
    2.3.3 Randomly assembled saturated communities are rarely feasible .... 14
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.3.4</td>
<td>Maximal ecological diversity</td>
<td>14</td>
</tr>
<tr>
<td>2.3.5</td>
<td>Community saturation</td>
<td>16</td>
</tr>
<tr>
<td>2.3.6</td>
<td>Diversity of top-down vs. bottom-up community assembly</td>
<td>16</td>
</tr>
<tr>
<td>2.3.7</td>
<td>Trait dispersion of randomly assembled communities</td>
<td>18</td>
</tr>
<tr>
<td>2.3.8</td>
<td>Transient extinction</td>
<td>20</td>
</tr>
<tr>
<td>2.4</td>
<td>Discussion</td>
<td>20</td>
</tr>
</tbody>
</table>

3 Evolution to alternative levels of stable diversity leaves areas of niche space unexplored  

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1</td>
<td>Introduction</td>
<td>22</td>
</tr>
<tr>
<td>3.2</td>
<td>Models and methods</td>
<td>22</td>
</tr>
<tr>
<td>3.2.1</td>
<td>Ecological Dynamics</td>
<td>24</td>
</tr>
<tr>
<td>3.2.2</td>
<td>Evolutionary Dynamics</td>
<td>26</td>
</tr>
<tr>
<td>3.2.3</td>
<td>Stability</td>
<td>27</td>
</tr>
<tr>
<td>3.2.4</td>
<td>Individual-Based Model</td>
<td>28</td>
</tr>
<tr>
<td>3.3</td>
<td>Results</td>
<td>29</td>
</tr>
<tr>
<td>3.3.1</td>
<td>Symmetric competition</td>
<td>29</td>
</tr>
<tr>
<td>3.3.2</td>
<td>Red Queen dynamics</td>
<td>31</td>
</tr>
<tr>
<td>3.3.3</td>
<td>Alternative metastable diversity</td>
<td>31</td>
</tr>
<tr>
<td>3.3.4</td>
<td>Large mutations</td>
<td>34</td>
</tr>
<tr>
<td>3.3.5</td>
<td>Finite populations</td>
<td>36</td>
</tr>
<tr>
<td>3.3.6</td>
<td>Small populations</td>
<td>38</td>
</tr>
<tr>
<td>3.4</td>
<td>Discussion</td>
<td>39</td>
</tr>
</tbody>
</table>

4 Adaptive diversification and niche packing on rugged fitness landscapes  

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.1</td>
<td>Introduction</td>
<td>43</td>
</tr>
<tr>
<td>4.2</td>
<td>Model</td>
<td>43</td>
</tr>
<tr>
<td>4.2.1</td>
<td>Tunable rugged landscapes</td>
<td>44</td>
</tr>
<tr>
<td>4.2.2</td>
<td>Ecological dynamics</td>
<td>46</td>
</tr>
<tr>
<td>4.2.3</td>
<td>Evolutionary dynamics</td>
<td>46</td>
</tr>
<tr>
<td>4.3</td>
<td>Results</td>
<td>47</td>
</tr>
<tr>
<td>4.3.1</td>
<td>Saturated ecological diversity</td>
<td>47</td>
</tr>
<tr>
<td>4.3.2</td>
<td>Adaptive diversification</td>
<td>47</td>
</tr>
<tr>
<td>4.4</td>
<td>Discussion</td>
<td>49</td>
</tr>
</tbody>
</table>

5 Rethinking the evolution of specialization: A model for the evolution of phenotypic heterogeneity  

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1</td>
<td>Introduction</td>
<td>53</td>
</tr>
<tr>
<td>5.2</td>
<td>Methods</td>
<td>53</td>
</tr>
<tr>
<td>5.2.1</td>
<td>Model Description</td>
<td>56</td>
</tr>
</tbody>
</table>
5.2.2 Equations .................................................. 60
5.2.3 Evolutionary Analysis ................................. 60
5.2.4 Evolutionary Simulations ............................. 62
5.3 Results ...................................................... 63
  5.3.1 Deterministic Evolution ............................. 64
  5.3.2 Branching ............................................. 64
  5.3.3 Evolutionary Simulations ........................... 64
  5.3.4 Mutation Size ....................................... 65
  5.3.5 Cost to Heterogeneity ............................. 65
  5.3.6 Unequal Resources .................................. 66
  5.3.7 Cross-feeding ....................................... 67
  5.3.8 Variable Environment ............................. 68
5.4 Discussion ................................................. 69

6 Conclusion .................................................. 74
  6.1 Chapter specific conclusions ........................... 74
    6.1.1 Chapter 2 ........................................... 74
    6.1.2 Chapter 3 ........................................... 75
    6.1.3 Chapter 4 ........................................... 76
    6.1.4 Chapter 5 ........................................... 77
  6.2 Future directions ....................................... 78
    6.2.1 High dimensional competition ..................... 78
    6.2.2 Horizontal gene transfer ........................... 79

Bibliography .................................................. 80

Appendices

A Supplementary information for Chapter 2 .................. 96
  A.1 Feasibility of random species ........................ 96
    A.1.1 Universal scaling of feasibility probability .... 96
  A.2 Results of Statistical Test for Trait Dispersion in One Dimension .... 97
  A.3 Supplementary figures ................................. 97

B Supplementary information for Chapter 3 .................. 106
  B.1 Full Model Details .................................... 106
    B.1.1 Ecological Dynamics ............................. 106
    B.1.2 Adaptive Dynamics ................................ 107
    B.1.3 Individual-Based Model ........................... 109
  B.2 Numerical stability analysis ......................... 109

viii
List of Tables

Table 5.1 Definitions of patterns of expression. ............................. 53
Table 5.2 Parameters and variables. ............................................. 58
Table A.1 Statistical test for trait dispersion in one dimension. ............. 98
Table B.1 Parameters and variables used to generate adaptive dynamics data
                                 and figures. ....................................................... 114
Table B.2 Parameters and variables used to generate individual-based model
                                 data and figures. ....................................................... 114
Table B.3 Parameters and variables used to generate partial differential equation
                                 model data and figures. .................................................. 114
Table B.4 Default asymmetric competition parameters. ........................ 115
# List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Evolutionary Stable States.</td>
<td>12</td>
</tr>
<tr>
<td>2.2</td>
<td>Example of 1D ecological and evolutionary stable states.</td>
<td>13</td>
</tr>
<tr>
<td>2.3</td>
<td>Final stable diversity and saturation of a randomly assembled community.</td>
<td>15</td>
</tr>
<tr>
<td>2.4</td>
<td>Initial saturation of a randomly assembled community necessary for the saturation of the final community.</td>
<td>17</td>
</tr>
<tr>
<td>2.5</td>
<td>Top-down versus bottom-up community assembly.</td>
<td>18</td>
</tr>
<tr>
<td>2.6</td>
<td>Evenness of randomly assembled communities in niche space.</td>
<td>19</td>
</tr>
<tr>
<td>3.1</td>
<td>Carrying capacity functions.</td>
<td>25</td>
</tr>
<tr>
<td>3.2</td>
<td>Stable states for symmetric competition with quartic and radially symmetric carrying capacity.</td>
<td>30</td>
</tr>
<tr>
<td>3.3</td>
<td>Asymmetric competition can lead to Red Queen dynamics.</td>
<td>32</td>
</tr>
<tr>
<td>3.4</td>
<td>Invasion fitness landscapes for alternative metastable states.</td>
<td>33</td>
</tr>
<tr>
<td>3.5</td>
<td>Levels of metastable diversity.</td>
<td>34</td>
</tr>
<tr>
<td>3.6</td>
<td>Large mutations allow escape from low diversity met-stable states.</td>
<td>35</td>
</tr>
<tr>
<td>3.7</td>
<td>Large mutations can cause transitions between locally stable levels of diversity.</td>
<td>36</td>
</tr>
<tr>
<td>3.8</td>
<td>Alternative metastable states for different levels of final diversity in individual-based simulations.</td>
<td>37</td>
</tr>
<tr>
<td>3.9</td>
<td>Finite population reduces realized diversity.</td>
<td>39</td>
</tr>
<tr>
<td>3.10</td>
<td>Finite population size can cause transitions in level of diversity due to demographic stochasticity.</td>
<td>40</td>
</tr>
<tr>
<td>4.1</td>
<td>Examples of rugged carrying capacity landscapes with ESS populations.</td>
<td>48</td>
</tr>
<tr>
<td>4.2</td>
<td>Ecological diversity as a function of the local ruggedness.</td>
<td>49</td>
</tr>
<tr>
<td>4.3</td>
<td>Evolutionary diversity as a function of the width of local ruggedness.</td>
<td>50</td>
</tr>
<tr>
<td>5.1</td>
<td>Evolution of resource specialization.</td>
<td>54</td>
</tr>
<tr>
<td>5.2</td>
<td>Metabolic constraint curves.</td>
<td>57</td>
</tr>
<tr>
<td>5.3</td>
<td>Beta distribution.</td>
<td>59</td>
</tr>
<tr>
<td>5.4</td>
<td>Selection gradient.</td>
<td>63</td>
</tr>
<tr>
<td>5.5</td>
<td>Evolutionary trajectories.</td>
<td>65</td>
</tr>
</tbody>
</table>
Acknowledgements

I would like to express my sincerest thanks to my supervisor Dr. Michael Doebeli for your tremendous support and guidance throughout this entire process. I would also like to thank my coauthor, Dr. Yaroslav Ispolatov. You have been both a great friend and colleague. Thank you to Gil Henriques and the other members of the Doebeli lab for all the engaging, challenging, and fun discussions. Lastly, thank you to my partner, Christine, and my parents for your love, support, and patience.
Chapter 1

Introduction

The truth of the principle, that the greatest amount of life can be supported by great diversification of structure, is seen under many natural circumstances. In an extremely small area, especially if freely open to immigration, and where the contest between individual and individual must be severe, we always find great diversity in its inhabitants.


Explaining the continued coexistence of many competitive species has long been one of the central aims of ecological and evolutionary theory. When Darwin wrote *On the Origin of Species* in 1859 [29] he introduced the idea that natural selection is the mechanism driving adaptation and the emergence of diversity in natural populations. While Darwin’s theory of natural selection became the unquestioned foundation of evolutionary theory, the nuances of how diversity emerges and is maintained has remained the focus of vigorous research and debate to this day.

The concept of an ecological niche, defined by G. E. Hutchinson as the environmental conditions that allow for the viability of a given species [77], has been at the center of ecological theory (and controversy) for over a century [134]. Following directly from this notion of a niche and Darwin’s theory of the survival of the fittest, the principle of Competitive Exclusion states that “complete competitors cannot coexist” [63]. When given sufficient time, the fittest of two competitors in the same environment will likely out-compete the other and drive it extinct. Darwin successfully used this logic to introduce the theory for how variation can be generated in the natural world through natural selection. However, a vast diversity of species seemingly compete for a limited amount of resources, yet still coexist. This conundrum, famously christened by Hutchinson The Paradox of the Plankton [78], implies the existence of more complicated dynamics and theories necessary to explain the extraordinary diversity in the natural world.

Indeed, classical theories of evolutionary dynamics only further reinforce this issue. The original formalization of evolutionary dynamics theory into a quantitative theory, spearheaded by Ronald Fisher, Seward Wright, and J. B. S. Haldane in the early 20th century, was a brilliant synthesis of Mendelian genetics and Darwinian natural selection [136]. However, these classical population genetics theories focused on explaining the change in frequency of genes with a given fitness. Because fitness is generally defined as a static attribute of
the gene, evolution via natural selection resembles an optimization process, with continual selection toward the genes with the highest fitness and thus best suited to the environment. However, this optimization process does not allow for the emergence or maintenance of diversity in an explicit way. Instead, based on an optimization of fitness, both diversification and the stable maintenance of diversity (as opposed to stochastic or transient coexistence) depend on the geographic isolation of competitors. Speciation occurs when a population is physically separated, at which point the optimization and adaptation to the now unique environments drives the diversification. Any additional diversity within the distinct locations now faces the same problem of optimization toward the most fit traits in that location and requires additional reproductive isolation.

Robert MacArthur and Richard Levins re-framed the concept of a niche into a dynamic property of the population that represents the distribution of the utilization of a resource laid out on a continuous axis (of one or more dimensions) [103]. In this framework, the competition for resources will lead to the natural partitioning of the niche axis by the population present into distinct niches. Allowing the fitness of an individual to be an emergent property of the population (i.e., frequency dependent), rather than a static number, coexistence is now simply a matter of “limiting similarity” of competitive traits (e.g., traits that govern resource utilization, space needed, etc.) to other competitors in the population. The stable coexistence of multiple types in the population is now theoretically supported. Indeed, frequency dependence is not simply a theoretical tool, it is pervasive in nature. Any competition for a limited resource (e.g., food, light, space) is by nature frequency dependent as resources used by one individual cannot be used by another. Thus the fitness of each individual must be a function of how many others require that same resource.

This same thinking has been expanded into evolutionary timescales to explain sympatric speciation, i.e., speciation that occurs without geographic separation. John Maynard Smith recognized the centrality of frequency dependence to evolutionary theory, creating evolutionary game theory [109, 110]. Evolutionary game theory was later extended to consider continuous trait spaces in a modelling framework called adaptive dynamics [33, 36, 114]. Perhaps most importantly, adaptive dynamics can be derived from individual dynamics when assuming small and rare mutations and large population size [18, 33]. Thus, rather than describing evolution in a purely phenomenological way, adaptive dynamics is derived from ecological dynamics. These theories based on frequency-dependent selection (niche-packing for ecological dynamics, evolutionary game theory and adaptive dynamics for evolutionary dynamics) provide a mathematical methodology to describe the generation and maintenance of coexistence between species.

Some of the most iconic and best-studied cases in the evolutionary biology literature are excellent as examples of adaptive diversification and niche partitioning. Darwin’s finches, the 18 species of finches he described during his voyage to the Galapagos Islands, have a distribution of beak size that corresponds to the size of the seeds or other food that
species feeds on [13]. The *Anolis* lizard of the Caribbean islands are found on both islands with one species of lizard and islands containing two species [summarized by 142]. As a single trait example among many, the islands with two species of Anoles house one species that is considerably larger and one considerably smaller than any of the species that live alone [142]. More recently, genetic evidence presented by Schluter [151, 153] shows that limnetic-benthic pairs of Sticklebacks in lakes in British Columbia evolved as a result of frequency-dependent resource competition.

### 1.1 Thesis goals

In this thesis I will continue to research these classic questions of how the diversity of species in natural communities emerges and is then maintained through evolutionary processes. Despite decades of foundational research into niche-packing and adaptive diversification, because of the complexity of natural communities, much is still left unexplained. Here I will present four chapters, each presenting a model and results representing an unresolved piece of the puzzle. As a whole, these chapters will discuss themes relating to the maintenance of diversity on ecological versus evolutionary timescales, the presence of alternative stable communities in the same environment, the effects of population size on the diversity of a community, when patterns in biodiversity are more likely explained by ruggedness in the fitness landscape or due to competition and limiting similarity, and the circumstances diversification dynamics may be supplanted by the evolution of non-heritable variation (i.e., phenotypic heterogeneity). Together, I hope these chapters will provide an interesting discussion into the adaptive diversification and community assembly dynamics of diverse ecological communities and build on the venerated body of theory concerning the emergence and maintenance of biodiversity in the natural world.

The specific goals of each of the four chapters are listed below.

### 1.2 General modelling approach

Chapters [2-4] describe a model based on the classical Lotka-Volterra ecological dynamics – the same basic theoretical framework used by Hutchinson in his definition of competitive exclusion. Species are defined by a phenotype (in one or more dimensions) that determines both the carrying capacity (the equilibrium population size of that species when alone) as well as the strength of the competitive interactions with other members of the community. Ecological dynamics can thus be described as a simple system of ordinary differential equations (ODEs). This is one of the most enduring and recognizable models in ecological theory, a testament to its usefulness both as a theoretical tool and simple description of natural populations.

I model evolutionary dynamics using different simulation techniques based on the princi-
amples of adaptive dynamics [33, 36, 113]. Adaptive dynamics is a continuation of evolutionary game theory [109] to continuous rather than discrete traits. Using a few basic assumptions (most importantly small and rare mutations), the adaptive dynamics framework provides a convenient tool for studying evolutionary and diversification dynamics that are an emergent property of the underlying ecology. Based on the specific question, I use various analytical and simulation techniques to implement the evolutionary dynamics including ODE and partial differential equation (PDE) implementations of the adaptive dynamics, individual-based models, and simpler ecological simulations that include mutations.

1.2.1 Note on stability

Studying the stability of ecological communities has a long history in both ecological [108] and evolutionary [44, 109] literature. As the work presented here investigates ecological communities on both ecological and evolutionary timescales, it is important to clarify the difference between ecological and evolutionary stability. Ecological stability refers to a community in which the population size of each species present remains constant and resistant to small perturbations. Evolutionary stability refers to a community in which the genetic composition of the species present are maintained by natural selection and similarly resistant to small perturbations. Neither form of stability is a necessary condition for the other.

Chapters 2–4 deal only with competitive communities (i.e., predation, mutualism, commensalism, and parasitism are not considered) modelled by Lotka-Volterra ecological dynamics and always result in a globally stable ecological equilibrium (i.e., the population sizes of the species present in the equilibrium community always converge to their equilibrium values regardless of their initial population sizes). Chapter 3 compares scenarios with both stationary and cyclic evolutionary dynamics. Chapters 2 and 4 both assume symmetric competition, which always results in stable evolutionary dynamics. Chapter 5 is modelled using more biologically explicit resource dynamics. While I largely consider a scenario that results in stable ecological dynamics, I also briefly introduce the scenario when resources are introduced to the system periodically, resulting in periodic fluctuations in population size. Regardless of the nature of ecological dynamics, this model also always results in stable evolutionary dynamics.

I would like to briefly recognize that there has been reasonable criticism for the overreliance on stable dynamics for ecology and evolutionary theory [68]. While I very much appreciate the importance of non-stable dynamics (see Chapter 3 for a discussion of diversity in systems with non-stable, Red Queen evolutionary dynamics), understanding the already complex systems with the simpler stable ecological or evolutionary dynamics is essential to developing an intuition for more complex systems and builds a foundation to extend theory further.
1.2.2 Remarks on the definition of species

Throughout this thesis, I will somewhat interchangeably use the terms ecotypes (or just types) and species. While there is serious debate and confusion surrounding the definition of species [111, 135], I use the term here simply as a synonym of ecotype and to refer to any distinct group of genetically similar individuals, roughly in-line with the genetic species concept [7]. As all the models presented here assume asexual reproduction, I feel the perhaps liberal use of the word species is both valid and more importantly, helps ground the theories presented here to the larger discussion on the evolution and ecology of biodiversity.

1.3 Chapter 2

One of the oldest and most persistent questions in ecology and evolution is whether natural communities tend to evolve toward saturation and maximal diversity. Robert MacArthur’s classical theory of niche packing [102, 104] and the theory of adaptive radiations [152] both imply that populations will diversify and fully partition any available niche space. However, the saturation of natural populations is still very much an open area of debate and investigation. While investigations of the diversity of evolutionary stable states (ESSs) are widespread, the diversity of communities that have yet to reach an evolutionary endpoint is poorly understood.

In Chapter 2, I use Lotka-Volterra dynamics and trait-based competition to compare the diversity of randomly assembled communities to the diversity of the ESS. I show that, with a large enough founding diversity (whether assembled at once or through sequential invasions), the number of long-time surviving species exceeds that of the ESS. However, the excessive founding diversity required to assemble a saturated or super-saturated community increases rapidly with the dimension of phenotype space. Additionally, traits present in communities resulting from random assembly are more clustered in phenotype space compared to random, though still markedly less ordered than the ESS. By combining theories of random assembly and ESSs I bring a new viewpoint to both the saturation and random assembly literature.

1.4 Chapter 3

In Chapter 3, I continue to investigate the question of community saturation through an evolutionary lens. While in Chapter 2 I compare the diversity of randomly assembled communities on ecological and evolutionary timescales, for simplicity competition was assumed to be symmetric, which necessarily results in stationary evolutionary dynamics and a single, global ESS [71]. However, recent evolutionary theory suggests the existence of alternative evolutionary stable states [17, 88, 176], which implies that some stable communities may not be fully saturated.

In Chapter 3 I use models based on the same Lotka-Volterra ecological dynamics and
three formulations of evolutionary dynamics (a model using adaptive dynamics, an individual based model, and a partial differential equation model) to investigate whether adaptive radiations tend to lead toward saturated communities in which no new species can invade or remain trapped in alternative, lower diversity stable states.

I show that with asymmetric competition and small effect mutations, following an adaptive radiation, non-stationary evolutionary dynamics (Red-Queen dynamics) can trap communities in low diversity states when limited by mutations of small phenotypic effect. These low diversity metastable states can also be maintained by limited resources and finite population sizes. Thus, limited resources not only reduces community population sizes, but also reduces community diversity, denying the formation of saturated communities and stabilizing low diversity, non-stationary evolutionary dynamics. When small mutations and finite populations are considered together, it is clear that despite the presence of higher-diversity stable states, natural populations are likely not fully saturating their environment and leaving potential niche space unfilled.

1.5 Chapter 4

In Chapter 4 I examine the question of community diversity by considering perhaps the two most commonly used theories in ecological theory to explain diversity in the natural world: rugged fitness landscapes and niche packing. Rugged fitness landscapes are used to explain diversity through the presence of local peaks, or adaptive zones, in the fitness landscape acting as available niches for different species. Alternatively, niche-packing and theories based on limiting similarity describe frequency-dependent selection leading to the organic differentiation of a continuous phenotype space into multiple coexisting types.

In Chapter 4 I synthesize these two theories into a single mathematical model. By combing rugged carrying capacity landscapes with frequency-dependent selection, I am able to investigate the effects of ruggedness on adaptive diversification and stably maintained diversity. I show that while increased ruggedness often leads to a decreased opportunity for adaptive diversification, it is the shape of the global carrying capacity function, not the local ruggedness, that determines the diversity of the ESS and the total diversity a system can stably maintain.

1.6 Chapter 5

While in the previous chapters I only consider traits that are genetically heritable (i.e., offspring inherits the phenotype of the parent, apart from the effects of any mutations), that is clearly a simplification of natural biological systems. To test this simplification, in Chapter 5 I investigate the circumstances non-heritable variation in a given trait (i.e., when an offspring’s phenotype is not determined by the phenotype of its parent) evolves in the place
of genetic variation in the population, when that trait is under diversifying selection. To answer this question, I consider phenotypic heterogeneity, which refers to genetically identical individuals that express different phenotypes. Traditionally, “bet-hedging” in fluctuating environments is offered as the explanation for the evolution of phenotypic heterogeneity. However, there are an increasing number of examples of microbial populations that display phenotypic heterogeneity in stable environments.

In this chapter I present an evolutionary model of phenotypic heterogeneity of microbial metabolism and a resultant theory for the evolution of phenotypic versus genetic specialization. I use two-dimensional adaptive dynamics to track the evolution of the population phenotype distribution of the expression of two metabolic processes with a concave trade-off. Rather than assume the commonly used Gaussian phenotype distribution, I use a Beta distribution that is capable of describing genotypes that manifest as individuals with two distinct phenotypes. This methodology allows me to describe two populations, both comprised of individuals with the identical distribution of phenotypes, but in one population those phenotypes are heritable, while in the other they are not.

In doing so, I find that environmental variation is not a necessary condition for the evolution of phenotypic heterogeneity, which instead can evolve as a form of specialization in a stable environment. I will explain that there are two competing pressures driving the evolution of specialization: directional selection toward the evolution of phenotypic heterogeneity and disruptive selection toward genetically determined specialists. Because of the lack of a singular point in the two-dimensional adaptive dynamics and the fact that directional selection is a first order process, while disruptive selection is of second order, the evolution of phenotypic heterogeneity dominates and often precludes speciation. I find that branching, and therefore genetic specialization, occurs mainly under two conditions: the presence of a cost to maintaining a high phenotypic variance or when the effect of mutations is large.
Chapter 2

Ecological diversity exceeds evolutionary diversity in model ecosystems

2.1 Introduction

The long-term diversity of competitive communities has been a focus of ecological theory since MacArthur’s seminal work on species packing and limiting similarity of competing species in a continuous trait space \[102,104\]. One of the enduring concepts to come out of this work is the question of whether natural communities are saturated (a community which is globally uninvasible) \[107\]. In the extensive species packing literature, the diversity of ecological communities are usually studied once a population reaches an evolutionary equilibrium, which naturally implies that the communities are saturated.

While it is undeniably important to understand the patterns of “niche-packed,” saturated equilibrium, these ESSs (evolutionary stable states) represent the endpoint of evolutionary dynamics \[36,44\] or the assembly of communities based on an infinitely diverse initial population. It has become more evident in recent years that evolutionary theory largely focusing on equilibrium dynamics is often limiting. Natural populations likely exist in non-equilibrium states \[126\], whether because of transient ecological dynamics \[50,74,126,149\], continually changing abiotic conditions \[72,90,164\], or simply because an evolutionary stable state has not yet been reached. Therefore, it is important to study patterns of diversity for newly assembled communities of various sizes in relation to the robust theory surrounding species-packed, saturated equilibrium.

Notably, while niche-packed equilibrium and the existence of a continuous distribution of species in trait space \[e.g., 94,143\] have been used as explanations for the “paradox of the plankton,” it has been repeatably shown that these coexistence continua are structurally unstable \[71,95,166\]. In all structurally stable formulations of the competitive exclusion model, communities with distinct species (as defined by their phenotype) are expected.

The importance of studying randomly assembled communities as a proxy for natural ecosystems was first appreciated by Robert May \[108\]. May was able to determine the stability of large communities when species interactions were defined by random interaction matrices \[108\]. Random matrix theory has continued to be productive in helping to under-
stand the ecological stability \[5, 6, 48, 93\] and feasibility (when there is a stable coexistence of all species in the community – i.e., no species in the community go extinct) of large communities \([11, 42, 156, 161]\). However, for these types of models, by directly defining species based on a random interaction matrix, rather than allowing interactions to be an emergent property of trait-based competition, community saturation can only be defined in the context of the species present in the interaction matrix. When instead defining species interactions by trait-based competition, community saturation becomes a characteristic of the ecosystem as well as the species present. A phenotype-based competition function is not only more realistic than randomly generated interaction matrices as the phenotypic competition introduces mechanistically-justified correlations into the interaction matrix (as the first-level approximation beyond the completely random matrix), it also allows us to have a clear picture of the evolutionary dynamics and to compare ecologically assembled diversity to the evolutionary stable state (ESS) produced by such an evolution.

Here, we use classic Lotka-Volterra ecological dynamics with species interactions defined by competition in an \(n\)-dimensional trait space to investigate the feasibility and stable diversity emerging from randomly assembled communities. We compare the emergent diversity of these random communities to the niche-packed, saturated evolutionary equilibrium for that system. The main question we address is how diverse of a randomly assembled founding population is required to result in a stable community with at least the same diversity as the ESS. We follow up by comparing the emergent diversity from different types of assembly processes and investigating how efficiently randomly assembled communities divvy up the available niche space.

2.2 Methods

2.2.1 Ecological Dynamics

In order to answer these questions we use a model based on classic Lotka-Volterra ecological dynamics with a \(d\)-dimensional phenotype, \(\vec{x}\), to determine a species’ carrying capacity and competitive ability. For simplicity we set the intrinsic growth rate of each species, \(r = 1\) and only consider symmetric competition \((\alpha(\vec{x}, \vec{y}) = \alpha(\vec{y}, \vec{x}) \forall \vec{x}, \vec{y})\). While these are both significant simplifications of the dynamics, they are reasonable, and oft-used, assumptions to facilitate an initial understanding of these dynamics.

The carrying capacity of each species is defined as \(K(\vec{x}) = \exp\left(-\frac{x^4}{4\sigma_K}\right)\) and species competition is modeled by a Gaussian competition function, \(\alpha(\vec{x}, \vec{y}) = \exp\left(-\frac{(\vec{x} - \vec{y})^2}{2\sigma^2}\right)\). Therefore, \(\alpha(\vec{x}, \vec{x}) = 1\) and \(\alpha(\vec{x}, \vec{y})|_{\vec{x} \neq \vec{y}} < 1\). Together the ecological dynamics for species \(i\) in a population of \(H\) total species are as follows:

\[
\frac{dN_i}{dt} = rN_i \left(1 - \sum_{j=1}^{H} \left(\frac{N_j \alpha(\vec{x}_i, \vec{x}_j)}{K(\vec{x}_i)}\right)\right)
\]
Here we chose to use a Gaussian competition function and a quartic carrying capacity function ($\sigma_\alpha = 0.6, \sigma_K = 1$ unless otherwise noted). This system is a commonly used model to study diversification [39, 40] and the same modelling framework used in Chapters 3 and 4. This model is a mathematically simple and structurally stable description of diversification dynamics. Using a higher order carrying capacity (and thus comparatively flat-shaped) function compared to the competition kernel both naturally restricts the viable phenotype space to an area around the origin (roughly between $-2$ and $2$ for the parameters chosen) and guarantees the presence of a branching point at the origin [9, 36], regardless of the choice of $\sigma_\alpha$. Moreover, using the quartic carrying capacity function avoids the structural instability of the more commonly used Gaussian carrying capacity function together with a Gaussian competition function, resulting in infinite branching [36, 133].

The ecological dynamics can be rewritten without the explicit phenotypes as

$$\frac{dN_i}{dt} = rN_i \left( 1 + \sum_{j=1}^{H} N_j \tilde{A}_{ij} \right)$$  \hspace{1cm} (2.2)

where the interaction matrix $\tilde{A}_{ij} = -\alpha(\tilde{x}_i, \tilde{x}_j)/K(\tilde{x}_i)$. This equation is the classical formulation of multi-species Lotka-Volterra dynamics where the interactive nature of the species are defined directly, rather than with explicit phenotypes. In a competitive community, like the systems we will study here, all elements of the interaction matrix, $A$, are negative. Including positive elements in an interaction matrix can be instead used to model more complicated systems including mutualistic or predatory relationships between species.

Of particular note, the symmetric competition function, $\alpha(x, y)$, we are using here does not mean that the resulting interaction matrix, $A$, need be symmetric and in practice it rarely is. However, as our competition function is indeed symmetric, there is a single globally stable equilibrium for any community [71], which in general includes finite and zero populations. Therefore, for symmetric competition an equilibrium population is the only possible outcome and no complex ecological dynamics (e.g., periodic or chaotic changes in population size) occur.

### 2.2.2 Ecological simulations

Communities were assembled by generating $H_0$ species, each with a randomly chosen phenotype $\tilde{x} \in (-2, 2)^d$. We were then able to solve for equilibrium population of the community by $\tilde{N}^* = -A^{-1}\tilde{r}$ (here, for simplicity we assume $\tilde{r} = 1$) and thus determine whether it is a feasible population if $N^*_i > 0 \ \forall i$. As mentioned above, the feasible equilibrium is always globally stable, so any feasible equilibrium represents the endpoint of the ecological dynamics.

However, if the randomly assembled community is not feasible, we are unable to analytically solve for the make-up of the final, stable population. Thus, we solved for the
final stable community by numerically integrating the system of ODEs using the Runge-Kutta-Fehlberg method. Each simulation was integrated until \( t = 10^{12} \). Any species with \( N_i < 10^{-8} \) was deemed extinct. The feasibility of the final simulated community was also calculated to determine if the ODE was run for enough time to reach a stable configuration.

### 2.2.3 Calculation of the ESS

In order to compare communities to the Evolutionary Stable State (ESS) for the given environment, evolutionary dynamics of each system were also calculated. Evolutionary simulations were accomplished using an adaptive dynamics framework. As the evolutionary dynamics are not a focus of this paper, and we are using a standard model and technique, the evolutionary dynamics will not be explained in further detail. Please see Chapter [3] or the source code for these simulations included in the supplementary materials for information on the adaptive dynamics of this system. Notably, while we used adaptive dynamics as we felt it was the fastest and most accurate way to determine the ESS of each system, a successive invasion simulation like the one used by [28, 138, 148] would deliver exactly the same ESS results.

### 2.3 Results

#### 2.3.1 ESS and Evolutionary dynamics

In order to find the saturation point of each system we simulated the ESS using adaptive dynamics. As mentioned above, because the carrying capacity function is of a higher order (i.e., flatter) than the competition kernel, there is always a branching point at the origin, regardless of the choice of \( \sigma_\alpha \). However, the presence of a branching point is not indicative of the diversity of the final populations. Using adaptive dynamics, the ESS was calculated for varying widths of the Gaussian competition kernel from \( \sigma_\alpha \in [0.35, 1.5] \). The ESS contains 2 species for any \( \sigma_\alpha \gtrsim 0.691 \), 3 species for \( 0.691 \gtrsim \sigma_\alpha \gtrsim 0.525 \), 4 species for \( 0.525 \gtrsim \sigma_\alpha \gtrsim 0.460 \), and an increasing diversity from there as \( \sigma_\alpha \) decreases.

With competition in dimensions \( d > 1 \), the ESS has the same values as the equivalent 1-dimensional system, with the species laid out approximately in an \( n \)-dimensional lattice hyper-cube. This results in the diversity of the ESS in \( n \)-dimensions equal to the ESS of the same parameterization in 1-dimension raised to the dimension. For the rest of the discussion we will focus on communities based on \( \sigma_\alpha = 0.6 \) corresponding to an ESS with diversity \( H_{ESS} = 3^d \) [e.g., Figs. 2.1, A.1].

#### 2.3.2 ESS is the endpoint of evolution

As mentioned above, the ESS represents the potential endpoint of the community on evolutionary timescales. Comparing the equilibrium diversity of communities on ecological and
Figure 2.1: **Evolutionary Stable States.** Evolutionary stable states were calculated using adaptive dynamics. Panel A shows the evolutionary dynamics over time and panel B the invasion fitness and ESS both for $\sigma_\alpha = 0.6$. Panel C is a diversification diagram showing the simulated ESSs for randomly chosen $\sigma_\alpha \in [0.35, 1.25]$. Adaptive dynamics simulations were run for $10^7$ time steps, including $10^5$ branching mutations. The species were then clustered using a K-means clustering algorithm with a minimum distance equal to 0.1. Due to computational complexity, small numerical errors remain for simulations with very small $\sigma_\alpha$. As noted in the text, these ESS are not particular to adaptive dynamics but could also have been generated using an algorithm of ecological dynamics including successive invasions of random species. ESSs in higher dimensions are comprised of the same trait values in 1 dimension laid out in an n-dimensional lattice. For a representation of the ESSs for $\sigma_\alpha = 0.6$ in 2 and 3-dimensions see Figure A.1.
evolutionary timescales can provide insight into natural populations that do not strictly exist in equilibrium. As nicely summarized by Edwards at al. [44], communities not at an ESS will experience selective pressure towards the ESS [however, see Chapter 3 and 39, 40, for discussions of non-equilibrium evolutionary dynamics]. In evolutionary time, supersaturated communities will likely experience the extinction of certain species and collapse to the ESS [e.g., Fig. 2.2]. Similarly, under-saturated communities represent ecological opportunity in the ecosystem which drives adaptive diversification toward the ESS [152].

Figure 2.2: Example of 1D ecological and evolutionary stable states. An example of ecological and evolutionary stable states for a randomly assembled population with one dimensional phenotype ($x$). Founding population contains 11 randomly chosen species. Panel A shows the population after $10^{12}$ time steps and their carrying capacities. Species that survived are shown in black and those that went extinct in red. The blue curve shows the invasion fitness (per capita growth rate of a small mutant) of the ecological stable community. Panel B shows the evolutionary dynamics and evolutionary stable state (ESS) with the same community after evolution (as simulated with adaptive dynamics) is run for 100 evolutionary time steps.

However, solely focusing on ESS minimizes the fact that evolution is ongoing. Studying ecological assembly processes has been a fundamental part of ecological theory [155], both to understand the founding of nascent communities as well as an analogy to constantly changing abiotic conditions and the opening of new ecological opportunities. Comparing the diversity emergent from a random assembly process to the diversity of the ESS ($H_{ESS}$), allows us to study the diversity of ecological communities before they reach an ESS.
2.3.3 Randomly assembled saturated communities are rarely feasible

When communities are made simply from a random assortment of competitive species (each species has a randomly chosen phenotype and competes in an $n$-dimensional trait space), saturated ($H = H_{ESS}$) or super-saturated ($H > H_{ESS}$) communities are almost never feasible [Fig. A.6]. At least one of the species will almost always go extinct. This follows simply from the theory of limiting similarity as there is a limited range of viable phenotypes. However, considering just the feasibility of random communities is fairly limiting as it does not allow for the natural assembly of stable communities through species invasion and extinction [98]. Thus, in order to determine the stable diversity ($H^*$) that results from a randomly assembled founding population, the ecological dynamics must be simulated.

For a longer discussion of the feasibility of randomly chosen species, including the effect of the dimension of the phenotype space on the probability of feasibility, please see Appendix A.1.

2.3.4 Maximal ecological diversity

We first consider the canonical case of “top-down” community assembly [156 161], where $N$ randomly selected species are placed together at a small population size and allowed to equilibrate to a stable community via numerical simulations of the Lotka-Volterra ecological dynamics.

As expected, as the diversity of the initial founding population ($H_0$) increases, so does the expected diversity of the final community ($H^*$) [Fig. 2.3]. However, this increase in expected feasible diversity is also clearly a sub-linear function, such that subsequent increases in founding diversity lead to a marginal increase in the diversity of the final community. While we make no mechanistic hypotheses to the specific shape of this diversity expectation curve, there is a visually proficient fit to a Michaelis-Menten regression [Fig. 2.3]. This is suggestive that the final diversity of a community is asymptotic as a function of the initial founding diversity, and therefore there being a maximal diversity possible for each system when communities are built through random assembly.

In one dimension the maximally feasible diversity is twice the ESS. This occurs when each species present in the ESS is replaced by two species, balanced on either side of the ESS species in phenotype space. The invasion of any third species with a similar phenotype will cause either one or both of those coexisting species to go extinct. While this can be confirmed analytically for a 1 species ESS, for higher diversity states it is confirmed by extensive numerical simulations.

In higher dimensions more complex, and dense, patterns of species in phenotype space are possible. It is not hard to manufacture very saturated communities comprised of species laid out in symmetric patterns (like hyper-spheres and hyper-cubes) surrounding each ESS point in phenotype space. The feasibility of these synthetic communities are all dependent
Figure 2.3: The final stable diversity and saturation of a randomly assembled community. Communities were assembled with random species in 1-5 dimensions. Ecological dynamics were run for $10^{12}$ time steps. Hollow points represent communities that did not stabilize to a feasible community by the end of the simulation and still contain at least one species that will eventually go extinct. Panel A shows the final diversity of communities as a function of their founding diversity. Grey lines are a regression using a nonlinear least squares fit to Michaelis-Menten form ($y = \frac{ax}{b+x}$). Regressions were fit only to communities that have stabilized by the end of the simulation. The Michaelis-Menten curves are not mechanistic, and were not chosen to model the ecological dynamics in any way, but are asymptotic curves (asymptote equal to regression parameter $a$) that are a good visual fit for the data. Panel B shows the saturation of the same communities as a function of the saturation of the founding community. Saturation is measured as the diversity divided by the diversity of the ESS ($H_{ESS} = 3^d$). Only communities with founding diversity of up to 500 species are displayed for panel A. For panel B communities were built with up to 500 species for dimension 1, 1500 for dimension 2, 2500 for dimension 3, and 5000 for dimensions 4 and 5.

on their symmetry in phenotype space and are extremely sensitive to small perturbations of the phenotypes present.

Notably, while our simulations resulted in an ever increasing final community diversity with increasing founding diversity, very large founding populations will likely equilibrate to the ESS, even without considering evolution. This is a scenario that was been studied often [148, 149] and is another method of numerically determining the ESS. However, we only saw high diversity assemblages result in the ESS for 1-dimensional simulations with $\sigma_{\alpha} = 1.0$ (in this case the $H_{ESS}=2$) despite simulating communities with a diversity over two orders of magnitude larger than the ESS [Fig. 2.3]. Thus, while the ESS is the theoretical high diversity limit of random assembly for an infinitely diverse founding population, such diverse
assembly processes that always result in the ESS are unlikely to play a role in the formation of natural communities.

2.3.5 Community saturation

To understand the pattern of the diversity of community assembly it is also important to consider the saturation (defined here as $H/H_{ESS}$) of both the initial and final communities in addition to just the diversity of these communities. In these randomly assembled communities, community saturation seems to asymptotically approach a maximal saturation of around two to three times the ESS for $d > 1$, regardless of dimension or niche width (defined by $\sigma_n$) [Fig. 2.3]. This suggests that while increasingly complex and dense patterns of coexisting species are easy to manufacture in higher dimensions, these patterns are unlikely to arise, at least with any significant frequency, via random assembly.

While randomly assembled communities have approximately the same maximal saturation regardless of dimension, creating a saturated or super-saturated community is increasingly difficult as dimension increases [Figs. 2.3, 2.4]. The median number of species needed to assemble a saturated community increases from 2.17 times the ESS for 1-dimension ($H_{ESS,d=1}=3$, median $H_{0,d=1}=6.5$ for saturated communities) to 10.7 times the ESS in 5-dimensional trait space ($H_{ESS,d=5}=243$, median $H_{0,d=5}=2597$ for saturated communities). This means that for 5-dimensional trait space 400 times the founding diversity is required to assemble a saturated community compared to communities competing in 1-dimensional trait space. As the diversity of the ESS continues to grow exponentially with higher dimensional trait space, the even greater founding diversity necessary in higher dimensions to assemble a saturated community becomes intractable very quickly.

2.3.6 Diversity of top-down vs. bottom-up community assembly

In addition to the top-down community assembly we describe above, we also consider community assembly from a bottom-up process. In a bottom-up assembly processes random species are added to the community sequentially, instead of placing all $N$ species in the system at once (top-down assembly) [27, 31, 155]. The community is initiated with two random species. Ecological dynamics are simulated for $10^{10}$ time steps or until the community stabilizes ($|dN_i/dt| < 9 \times 10^{-9}$ $\forall i$) at which point another randomly chosen species is added. The simulation ends when $N$ species (including the initial 2) have been added to the community.

Communities assembled from the bottom-up displayed roughly the same diversity expectations as those assembled from the top-down, except randomly-assembled bottom-up communities tend to be slightly less diverse than communities assembled from the top-down with the same number of species [Fig. 2.5].

Servan at al. [155] show that in competitive communities the community generated via a top-down assembly process can also always be reached sequentially (bottom-up) if drawing
Figure 2.4: Initial saturation of a randomly assembled community necessary for the saturation of the final community. Here we show the saturation (diversity divided by the diversity of the ESS) of the initial, randomly assembled communities that end up stabilizing at approximately (95% to 105% of saturation) the saturation point for the given system. To create a saturated community from a random assembly of species, a more saturated initial founding population of species is required as dimension increases. The boxplots show the median, first and third quartiles, as well as extreme values.

from the same species pool. However, multiple final, stable communities are possible with the same species pool. The priority effects and historical contingencies [21, 50] emergent from the specific order of invading species in a bottom-up assembly often results in an alternative stable community compared to one built top-down.

Here, the increased diversity in top down communities is likely because of complex patterns of species in phenotype space that require a specific order of species invasions to form sequentially [158]. These are configurations of species in which at least some of the pairwise combinations of species are unable to coexist in isolation but are stabilized by the presence of another species in the community. These multi-species consortia either have to be built up in a specific order of sequential species or can only exist when all species are present at the same time (e.g., via top-down assembly). Thus, despite the higher diversity community being accessible via a sequential assembly processes, some of the time bottom-up assembled communities get stuck in lower diversity stable communities.

However, as noted above, the diversity difference between the two assembly processes is fairly minor. Initial diversity and the dimension of competition are much stronger indicators of both final community diversity and saturation than the nature of the assembly processes. While we did not test other, more complicated assembly processes comprising of invasions with more than one species at a time [31, 59], it logically follows that the final diversity
Figure 2.5: **Top-down versus bottom-up community assembly.** Top-down communities were assembled by selecting $H_0$ random species and initiating ecological dynamics with all species together. Bottom-up communities were assembled sequentially one species at a time until $H_0$ species were allowed to invade the community. The ESS in one dimension is made up of 3 species and increases exponentially with dimension ($H_{ESS} = 3^d$). The grey lines are a regression using a nonlinear least squares fit to Michaelis-Menten form. Regressions were fit only to communities that have stabilized by the end of the simulation. The solid lines and squares represent bottom-up communities; dashed lines and circles are top-down.

of these communities will be somewhere in between those built in a purely top-down or bottom-up fashion.

### 2.3.7 Trait dispersion of randomly assembled communities

A key feature in species-packed equilibria are evenly spaced species in niche space to efficiently divvy up the available niche space [103, 112]. To investigate this we calculated the pairwise distances (in phenotype space) of each species to every other in the community. The “dispersion” of the community was then measured by the coefficient of variation (standard deviation divided by the mean) of the distance of each species to its nearest neighbor ($CV_{NN} = \sigma/\mu$) [10]. As the ESSs for these systems take the form approximately of an $n$-dimensional lattice (the distances between rows/columns of the lattice are not necessarily equal when the $H_{ESS} \geq 4^d$, with species near the origin being slightly closer together), these ESSs are very under-dispersed (more regularly spaced in trait space than would be expected at random). The coefficient of variation of the distance to the nearest neighbor separation in these lattice-like ESSs is equal to (in systems with an $H_{ESS} \leq 3^d$ as they form a hyper-cube in trait space) or close to (in communities with an $H_{ESS} \geq 4^d$) 0.
While randomly assembled communities were more dispersed in trait space than the lattice-like configuration of the ESS, they were also distinctly less dispersed than random configurations [Fig. 2.6]. This was further confirmed in one dimension by using Welch’s t-test to statistically assess the dispersion of both top-down and bottom-up communities versus random traits of the same diversity [Table A.1]. For both community assembly processes (top-down and bottom-up) and all levels of feasible diversity (3-6 species), the randomly assembled communities have significantly under dispersed traits by this measure compared to both uniformly and Gaussian distributed traits \((p < 0.05)\). This means that even without evolution, communities will self-organize to efficiently utilize the available niche space solely through the extinction of overlapping species.

Figure 2.6: **Evenness of randomly assembled communities in niche space.** The pattern of trait dispersion was measured for randomly assembled communities using the coefficient of variation of the distance to the nearest neighbor \((CV_{NN})\) for each species in the community. A value of \(CV_{NN} = 0\) corresponds to a perfectly ordered distribution of species, or a lattice in trait space. A very high \(CV_{NN}\) would correspond to a very disordered community that has little organized structure. Colors represent the method of community assembly with yellow and red representing top-down and bottom-up randomly assembled communities; green and blue are the null expectation of uniformly \((\in [-2, 2])\) and Gaussian distributed \((\mu = 0, \sigma = 1)\) traits. Bottom-up communities were built with up to 500 random species. Top-down communities were built up to 500 species for dimension 1, 1500 for dimension 2, 2500 for dimension 3, and 5000 for dimension 4 and 5. Ecological dynamics run for \(10^{12}\) time steps. Only communities that stabilized to a feasible community when the simulation was terminated are shown. Results for 1-5 dimensional trait spaces are shown in each panel.

Patterns of trait dispersion become especially clear as community saturation increases. As saturation increases, species become more and more evenly spaced in trait space. Inter-
estingly, at least for the sizes of communities we were able to simulate, the $CV_{NN}$ seems to approach $\approx 0.25$, for all dimensions greater than one. This is somewhat surprising, as it is easy to assume that communities become increasingly over dispersed as they become more saturated. However, it seems that in higher dimensions, completely symmetrical and even distributions of species are unlikely to form.

This finding of common under dispersion of traits in randomly assembled communities mostly corroborates [10], who found that in simulated communities of 51 species, those that have evolved due to competition are significantly more ordered compared to the null expectation. While they were unable to find a statistical significance, they also state that randomly assembled communities without evolution seemed under-dispersed than the null expectation.

Also of note, top-down and bottom-up communities of the same diversity were not found to differ in this measure of trait spacing. This means that while bottom-up assembly leads to a slightly less diverse community on average, once established, communities of a certain diversity are indistinguishable based on assembly process.

### 2.3.8 Transient extinction

We ran the ecological dynamics for an extremely long timescale ($10^{12}$ time steps) which ensured that almost all simulations eventually settled to a stable community. However, even after this long time, some communities did not yet stabilize. It is a known phenomenon that extinction can be “exceedingly slow” [74]. Scheffer and van Nes [149] found that extinction transients can cause the persistence of similar species causing “clumping” of species in trait space. We can confirm the same phenomena and thus unsurprisingly, very saturated communities, where there are significant numbers of very similar species, had the longest lasting transient extinction. For an example of the ecological dynamics of a single community with transient extinction please see Figure[A.5]

Not all cases of transient extinction were caused by the clumping of similar species. In rare cases nearly symmetric patterns of species in niche space, usually centered on a singular point in the ESS, resulted in a nearly “balanced” configuration and transient dynamics. however, these cases were rare and were not identified in many communities generated via random assembly.

### 2.4 Discussion

One central problem in ecology and evolutionary theory that has seen a resurgence in interest in recent years is understanding the characteristics of an ecosystem that lead to the coexistence of many species. Previous work on the topic has largely focused on the distribution of species at an ESS [e.g., 102], coexistence due to transient dynamics [149], or community assembly through the creation of random interaction matrices in the Lotka-
Volterra model framework [6][11]. Here we have shown that while the diversity of the ESS of a system is certainly important, communities built through random assembly can be both unsaturated or super-saturated compared to that ESS depending on the diversity of the random assembly. However, for every system as long as the founding community is diverse enough, the resulting community is all but guaranteed to be saturated or super-saturated. This is true for both top-down and bottom-up assembly processes (though communities created with a top-down processes are on average slightly more diverse than those create from the bottom up).

Perhaps most importantly, the founding diversity necessary to create a saturated community actually increases faster than the increase in the diversity of the ESS as dimension increases. This means in natural communities that are likely competing in high dimensional phenotype space [12] [40] [43] [79] [129], the generation of a saturated community through random assembly is essentially impossible. In higher dimension, evolution and frequency dependent selection are required to build saturated communities that efficiently divide trait space into regular niches. Even with very large founding diversity, communities built through random assembly retain some of the structural inefficiencies in trait dispersion from the complex and random assortment of species in comparison to the lattice-like ESSs. Both the difficulty in creating a saturated community and the more randomly dispersed trait patterns of randomly assembled communities reinforce the common trope in evolutionary literature that evolution is an incredibly efficient process in organizing species in trait space.

Asymmetric competition can lead to both more interesting ecological (unstable or cyclic coexistence [71]) and evolutionary dynamics in high dimensional phenotype space (e.g., the Red-Queen dynamics discussed in Chapter 3 or evolutionary chaos [40]), depending on the specific functional form of the competition kernel. While diversity patterns due to asymmetric competition is beyond the scope of this chapter, in Chapter 3 we show that in systems with non-stable (Red Queen) evolutionary dynamics randomly assembling super-diverse communities was possible, but exceedingly rare, creating a possible analogy to the difficulties in creating saturated communities with symmetric competition.
Chapter 3

Evolution to alternative levels of stable diversity leaves areas of niche space unexplored

3.1 Introduction

One of the fundamental goals of ecology is to understand how biodiversity is maintained. Competition theory predicts that two species with identical niches will lead to competitive exclusion and one will win out. Early theoretical work by Robert MacArthur [102–104] codified the idea that competition can lead to the partitioning of continuous phenotype space into niches, allowing for the stable coexistence of species. For species to stably coexist, selective pressures will limit similarity and partition species into individual niches.

MacArthur introduced the idea of niche packing as one of two ways of diversifying (the other being exploration) [104]. Niche packing implies that a higher density of species must lead to a greater partitioning of the available niche space. This has inevitably led ecologists to ask at what point communities will saturate with maximal diversity and whether natural communities tend to exist at saturation [65, 107, 137]. While this question has recently led to vigorous debate and research, there has been little theoretical treatment of the evolutionary dynamics for saturated versus unsaturated communities. For instance, it is a well known result that ecological stability does not necessarily imply evolutionary stability and that maximal ecological diversity is often evolutionarily unstable [44]. For a larger discussion of the saturation of ecological communities, see Chapter 2.

It has become increasingly clear that eco-evolutionary dynamics play a large role in the long-term maintenance of biodiversity. For example, adaptive radiations, the rapid ecological differentiation of a single clade [152], are able to generate vast amounts of diversity [4, 25]. Eco-evolutionary models of frequency-dependent competition with mutation have been used to show how adaptive radiations can emerge from these simple competitive interactions, leading to diversification and niche partitioning [32, 37].

Recent work has investigated the theoretical existence of alternative evolutionary stable states (ESSs – long-term endpoints of an evolutionary process), the presence of multiple different communities in a given system that are uninvadable by a mutant of small effect [17, 88, 176]. The presence of alternative ESSs necessarily implies that certain stable ecological
communities may not be at saturation. Certain ESSs may even be “Garden of Edens” that are unreachable by successive small mutations \cite{125} or are only reachable through rapid evolution that occurs on the same timescale as ecology \cite{88, 176}. Calcagno et al. \cite{17} create an atypical scenario running contrary to classical niche-partitioning reasoning, where the initiation of diversification is dependent on there already being diversity present. While both of these results are intriguing, the simple question of whether adaptive radiations tend toward saturated communities or stall at an unsaturated ESS remains largely unanswered.

Given the extraordinary complexity of biological processes, it is natural to think that selection takes place in many dimensions. Despite this, a majority of our intuition of evolutionary dynamics come from narratives of individual traits or models with single phenotypic dynamics. Recent studies of evolution in high-dimensional phenotype space show that evolutionary dynamics can often be complex \cite{39, 40}. With increasing dimension, low and intermediate levels of diversity are increasingly non-stationary, with periodicity most common in lower dimensions and chaos in high dimensions. As the community diversifies, evolutionary dynamics slow down, often, but not always, fully stabilizing \cite{40}. While the patterns that emerge are often stable, it is not yet clear whether these represent fully saturated communities or lower diversity ESSs. This question is essential for our understanding of how diversity is generated and maintained in natural communities.

Here we investigate whether different patterns of niche partitioning in multi-dimensional phenotype space can lead to alternate levels of stable diversity in a given system and whether adaptive radiations generally lead to saturated communities. We use an eco-evolutionary model with ecological dynamics described by the classic formulation of Lotka-Volterra competition and evolution as a trait substitution process in continuous phenotype space. For computational and visualization simplicity, only two-dimensional phenotypes are considered. The evolutionary dynamics are solved using three separate modeling frameworks: adaptive dynamics \cite{55}, individual-based simulations, and partial differential equations. All three models are run with the same ecological dynamics. Numerical simulations of the adaptive dynamics allow for the most efficient computation and most extensive exploration of the three modeling frameworks. The individual-based models allow us to test the assumptions of adaptive dynamics and explore the effects of finite population size and phenotype distributions on the patterns of adaptive radiations. Similarly, the PDE-based model, while computationally challenging, allows for a deterministic implementation that is able to consider within population variance and no mutation limitation assumption.

We will show that adaptive radiations in multiple dimensions often lead to locally stable levels of diversity. Higher diversity states and eventually globally stable community saturation may be reached either through large mutations, immigration of species with phenotypes novel to the community, or if the adaptive radiation was initiated with higher levels of standing genetic variation. With asymmetric competition, the lower diversity states often take the form of stable limit cycles that represent Red Queen dynamics \cite{173}. While these low
diversity states are only locally stable, finite population sizes further restrict diversification despite available niche space, stabilizing low diversity, unsaturated communities and, depending on the system, perpetuating Red Queen dynamics. These patterns of locally stable, low levels of diversity are likely present in nature, leaving communities unsaturated and areas of phenotype space open for invasion and continued adaptation. These results shed light on the speed and characteristics of adaptive radiations as well as whether or not diversity tends to evolve to saturation [107].

3.2 Models and methods

3.2.1 Ecological Dynamics

Here we examine a model of phenotypic evolution based on classic logistic Lotka-Volterra ecological dynamics. Individuals are defined by a two-dimensional continuous phenotype and population size. In a monomorphic population of a single phenotype \( \vec{z} \), the equilibrium density of that population equals the carrying capacity, \( K(\vec{z}) \), of that phenotype. We will use two different forms of carrying capacity functions, from now referenced to as quartic or radially symmetric [Fig. 3.1].

For the quartic case the more general \( d \)-dimensional carrying capacity function is

\[
K(\vec{z}) = \exp \left( - \sum_{k=1}^{d} \frac{z_k^4}{4} \right)
\]

(3.1)

The radially symmetric carrying capacity is

\[
K(\vec{z}) = \exp \left( - \frac{\left( \sum_{k=1}^{d} z_k^2 \right)^2}{2} \right)
\]

(3.2)

When evolution is considered, both these functions impose stabilizing selection on the phenotype towards the origin where the carrying capacity is maximal. Due to the higher order term in both of these functions, carrying capacity has a fairly “flat” peak, which naturally restricts viable phenotype space to approximately between \(-2\) and \(2\) in each dimension. In addition to naturally limiting viable phenotype space, using a quartic carrying capacity avoids the structural instability of a Gaussian carrying capacity and Gaussian competition kernel that results in infinite branching [36, 133].

Individuals compete with others governed by a competition kernel \( \alpha(\vec{z}_i, \vec{z}_j) \). The competition kernel equals 1 when an individual competes with another with the same phenotype and decreases to 0 as the phenotypic similarity of the two competing individuals decreases. Thus, similar individuals will have a greater effect on each other’s growth compared to individuals with more distinct phenotypes. We consider situations with both symmetric
Figure 3.1: **Carrying capacity functions.** Two carrying capacity functions in 2D trait space. The peak of both functions is 1 at the origin and decreases to 0 as the phenotype increases or decreases. The quartic carrying capacity has a square peak while the radially symmetric carrying capacity has a circular peak. As both functions are of order 4, they are “flatter” on top than a standard Gaussian distribution. For the individual-based simulations, the same carrying capacity functions are used, but multiplied by a scalar $K_{max}$ that determines carrying capacity in a number of individuals at the origin. This scalar controls the “richness” of the environment.

and asymmetric competition. Symmetric competition refers to when individuals impart exactly the same competition load on each other such that $\alpha(\vec{z}_i, \vec{z}_j) = \alpha(\vec{z}_j, \vec{z}_i)$. While this is traditional [36] and conceptually convenient, perfect symmetry rarely occurs in nature and asymmetric competition has been explicitly measured [70]. Therefore, we also consider asymmetric competition where $\alpha(\vec{z}_i, \vec{z}_j) \neq \alpha(\vec{z}_j, \vec{z}_i)$. For symmetric competition, the competition kernel takes the form of a Gaussian with variance equal to $\sigma^2_\alpha$. For asymmetric competition a term is added with coefficients $b$ that determine the nature of the competitive interaction between the phenotypes in the two dimensions. This asymmetric term is non-mechanistic and can be thought of as the first-order term in a Taylor expansion of some higher order asymmetric interaction function [39]. In this way, it is the simplest way to add asymmetry to Gaussian competition.

$$\alpha(\vec{z}_i, \vec{z}_j) = \exp \left( \sum_{k,l=1}^{d} b_{kl} (z_{ik} - z_{jl}) z_{il} - \sum_{k=1}^{d} \frac{(z_{ik} - z_{jk})^2}{2\sigma^2_\alpha} \right)$$

(3.3)
When the $b$ coefficients are set equal to 0, the function reduces to symmetric, Gaussian competition. The competition kernel provides the frequency-dependent component of the ecological dynamics, which allows for the stable coexistence of multiple competing phenotypes under certain conditions.

While the functional forms used here for carrying capacity and competition are largely phenomenological, they represent biologically reasonable scenarios \[36\] and are well supported in the literature \[36, 142\].

Based on the classic Lotka-Volterra formulation, ecological dynamics are thus:

$$\frac{dN_i}{dt} = rN_i(t) \left(1 - \sum_{j}^{M} \frac{\alpha(\vec{z}_j, \vec{z}_i)N_j(t)}{K(\vec{z}_i)}\right)$$

(3.4)

for growth rate $r$, a population $i$ with phenotype $\vec{z}_i$ and population size $N_i(t)$ that competes with each of $M$ other groups of individuals with distinct phenotypes $\vec{z}_j$, and population sizes $N_j(t)$.

For simplicity and computational tractability, all simulations are spatially homogeneous and positions of individuals or groups in space are ignored.

### 3.2.2 Evolutionary Dynamics

#### Adaptive Dynamics

We model evolution using adaptive dynamics. Adaptive dynamics allows for tractable computation of evolutionary dynamics when a few basic assumptions are met: (1) there is a 1-to-1 map from genotype to phenotype; (2) all genetically identical individuals can be represented as a single phenotype with no phenotypic variation (i.e., a delta function); (3) when a favorable mutation arises, it usually out-competes the resident, driving the resident extinct; and (4) mutations are small and rare. It is essential in the derivation of the adaptive dynamics that the resident populations are at their ecological equilibrium, or in other words, that population dynamics are infinitely fast on the evolutionary timescale and any mutant that arises either fixes in the population or goes extinct before another mutant is introduced.

To derive the adaptive dynamics, we must first define the invasion fitness \[\Pi_3\] $f(\vec{z}_r, \vec{z}_m)$ as the per capita birth rate of a rare mutant $m$ in the monomorphic population of resident $r$ that is at its ecological equilibrium population size $K(\vec{z}_r)$:

$f(\vec{z}_r, \vec{z}_m) = 1 - \frac{\alpha(\vec{z}_r, \vec{z}_m)K(\vec{z}_r)}{K(\vec{z}_m)}$.

When the invasion fitness is positive ($f(\vec{z}_r, \vec{z}_m) > 0$), the mutant can invade the resident population. When mutual invasibility occurs, i.e., the invasion fitness of the resident into an equilibrium population of the mutant is also positive ($f(\vec{z}_m, \vec{z}_r) > 0$), individuals of the two phenotypes can coexist indefinitely.

By taking the partial derivative of the invasion fitness function with respect to the mutant when the mutant phenotype equals the resident (mutations are infinitely small) we
can derive the selection gradient and then the canonical equation of adaptive dynamics, which describes the trajectory of a single, monomorphic population as it evolves in the trait space (which in our case is two-dimensional). A more detailed description of adaptive dynamics, please refer to Dieckmann and Law [33] and Doebeli [36].

**Speciation**

The canonical equation of adaptive dynamics, as introduced above (see Appendix B for a full derivation of the adaptive dynamics), can thus only describe the movement of populations in phenotype space, but not speciation or extinction events. Evolutionary branching is a well known phenomenon that occurs when there is an attracting equilibrium or nullcline [83, 84] (for further discussion of branching across nullclines see Chapter 5) in trait space that is also a fitness minimum [55]. To model these we use a well described algorithm [40] where the canonical equation of adaptive dynamics is numerically solved for some period of time at which a random population is chosen and a small mutant is introduced nearby. If that mutant is viable and is mutually invasible with its parent, the population successfully branched and the simulation continues with an additional phenotype. In doing so, this algorithm results in deterministic ecological dynamics and quasi-deterministic evolutionary dynamics in which evolutionary trajectories are deterministic but branching is stochastic.

**Simulations**

Evolutionary simulations are conducted thusly: (1) solve for the ecological equilibrium of the current population; (2) delete any populations that fall below a minimum viable population size and considered extinct ($10^{-8}$); (3) solve the canonical equation of adaptive dynamics for a fixed length of evolutionary time; (4) for computational speed, merge any two populations whose phenotypes are within a very small distance of each other ($\Delta z$); (5) introduce a mutant population, whose phenotype is a small deviation ($\epsilon_{mut}$) from the parent in a random direction; (6) delete the mutant if it cannot invade the population; and (7) repeat the process until an evolutionary stable community or a designated time has been reached. After each time step, similar phenotypes (those with phenotypes within a small distance from each other) are clustered into species as to better represent the number of distinct phenotypic groups alive at any given time (this does not affect the simulations and is only an accounting device).

**3.2.3 Stability**

Given the mathematical complexity of these dynamics, we were unable to analytically determine the evolutionary stability of the resulting communities. Instead, we define metastable evolutionary states, stationary or cyclic, as those, to which the system quickly converges and in which it resides much longer than the convergence time, possibly indefinitely. Mech-
anistically, the exit from a metastable state is conditional on significantly larger mutations than the convergence to it.

Our definition of metastability is in line with more common causes in physics and chemistry. Consider for example a well-studied problem of protein folding \([46]\): A model initiated with a completely disordered state quickly folds into one of potentially very many metastable conformations, and it takes long time or a potential guidance (assistance) from other proteins (chaperons) to reach the native functional fold. However, there is a subtle difference between metastability in ordering in physics and metastable states in evolution. In the physics systems, there usually exists a function, such as a free energy, that reaches its absolute minimum in the truly stable state, while the metastable states correspond to local minima, providing a very clear distinction between the former and the latter states. However, in essentially non-stationary systems, such as evolving systems, it is often impossible to define such a function.

### 3.2.4 Individual-Based Model

In order to examine how finite population size affects the evolutionary dynamics, we use an individual-based simulation. In these simulations, individuals have a fixed birth rate and a frequency-dependent death rate calculated from the carrying capacity and competition kernel as described above. Every time step a single individual is chosen to die or give birth to an offspring with phenotype equal to its parent plus a small mutation in a random phenotypic direction. Instead of a single phenotype describing each population of individuals, populations are now represented by a cloud of points in phenotype space. In order to determine distinct species, individuals are clustered such that every individual of a given “species” lies within a prescribed phenotypic distance to at least one other member of that species. This clustering is purely accounting and has no bearing on the dynamics. For a more detailed account of individual-based simulations and their relation to adaptive dynamics please see \[18, 19\] and \[82\].

The individual-based simulations are fully stochastic and do not require any of assumptions of adaptive dynamics except the 1-to-1 genotype-phenotype map. Thus, in addition to providing a means to investigate the effects of finite population size, these simulations also act as a check on the applicability of the assumptions required by adaptive dynamics. Additionally, unlike adaptive dynamics, evolutionary branching is an emergent property of the individual-based simulations \[18\] and acts as a further confirmation of diversification within the adaptive dynamics simulations.

For both adaptive dynamics and individual-based simulations the population is initially seeded with individuals with a randomly chosen phenotype between \(-2\) and \(2\) in each dimension, roughly coinciding with the area of viable phenotype space for both carrying capacity functions. Simulations were seeded with different numbers of individuals (between 1 and 100), each with a distinct phenotype, in order to investigate the effects of standing
genetic variation on the dynamics of adaptive radiation.

From here on we will refer to groups of phenotypically similar individuals as a species. In the individual-based model a species takes the form of a distinct cloud of points while in the adaptive dynamics simulations a species is represented by a single phenotype and its population size.

3.3 Results

Because the carrying capacity functions we investigate here both have a broader maximum at the origin than that of the Gaussian competition kernel, the origin is always the minimum of the invasion fitness and there necessarily exists a branching point at the origin. Thus the possibility of evolutionary coexistence between two or more phenotypes is guaranteed. In order to further encourage diversification, we only use $\sigma_0 < 1$, which would be the condition to generate a branching point at the origin if we had instead used carrying capacity functions of equal order to the competition kernel.

Unless otherwise noted, all figures were generated using parameters listed in Appendix B.

3.3.1 Symmetric competition

For symmetric competition ($b = 0$), a quartic carrying capacity, and $\sigma_0 = 0.5$, when starting with a single species (monomorphic population defined by its two dimensional phenotype), that species quickly evolves under directional selection toward the fitness maximum at the origin. Once there, it will start to successively branch, quickly stabilizing into an evolutionary stable community (ESC) with 16 species arrayed in a 4x4 grid [Fig. 3.2]. This pattern naturally emerges as the community evolves to pack the viable (and approximately square) niche space, while still maintaining space from neighboring species due to competition. For a more detailed discussion of the patterns and dynamics of species packing in multi-dimensional phenotype spaces please refer to [40].

With a radially symmetric carrying capacity, the story is largely the same, but instead of diversifying into a grid, the population arranges itself into two concentric circles. The invasion fitness along the ridges of these concentric circles is almost flat and nearly equal to 0. This resulted in nearly neutral selection along the ridges and different numbers of final species in each simulation, ranging from 24 to 34 between both circles [Fig. 3.2]. While the invasion fitness landscape in figure also indicates directional selection toward the origin, the invasion fitness at the origin is three orders of magnitude less than maximum invasion fitness during the initial adaptive radiation, indicating weak selection. Manually placing a population at or near the origin does result in a stable configuration, but diversification toward the origin is so slow it was nearly imperceptible during our simulations even when simulations were run for far longer than our results shown here. Like selection toward the origin, areas of slight positive invasion fitness on the concentric circles indicate that these
Figure 3.2: **Stable states for symmetric competition with quartic and radially symmetric carrying capacity.** Figures were generated using adaptive dynamics simulations. Points in the upper panels represent surviving species at the end of each simulation and the surface shows the invasion fitness (per capita growth rate of a rare mutant) with positive invasion fitness displayed in orange and negative in blue. The maximum invasion fitness for each panel is printed in the top right corner. When a symmetric competition kernel was used, simulations all converged on similar patterns regardless of the initial population. All simulations are run with the same parameters, which can be found in Table B.1.

configurations are likely not fully stable. Clusters on the outer ring seem to be slowly continuing to undergo diversification as long as the simulations were run, though the rate of speciation events and speed of evolution slowed dramatically as the rings filled up.

These simulations with the radially symmetric carrying capacity function and symmetric competition were the only simulations we ran that did not fully settle in stationary or cyclic configurations on timescales that were computationally feasible. Similar long-term transients were not found in any simulations with different functional forms for carrying capacity or competition, or with different parameterizations, so it is likely that this is a degenerate case caused by a perfectly radially symmetric carrying capacity function and Gaussian competition. Indeed, it is a well known result that in a one-dimensional trait space with a Gaussian carrying capacity kernel and symmetric, Gaussian competition, adaptive dynamics results in an infinite branching process [36]. However, like in our simulations, this “infinite branching” quickly degrades to discrete phenotypes when either the carrying capacity or competition kernels are altered from being perfectly symmetric.
3.3.2 Asymmetric competition can lead to Red Queen dynamics.

For certain values of the four $b$ coefficients (the coefficients that govern the nature of asymmetric competition) the population quickly settles into an evolutionary stable state (ESS). As mentioned in Doebeli et al. [40], in a two-dimensional system like the one simulated here, most randomly chosen $b$ values result in evolutionarily stable communities (ESCs). These configurations are often grid-like for the quartic carrying capacity or concentric circles for the radially symmetric carrying capacity but with some “skew” related to the asymmetry in competition. These ESCs can fully saturate the environment, leaving little to no area of trait space with positive invasion fitness [Fig. 3.2].

Other combinations of $b$ however, can result in non-equilibrium evolutionary dynamics. There is significant literature already detailing how asymmetric competition can lead to non-equilibrium dynamics – either stable limit cycles [92] or in higher dimensions, chaos [39, 40, 81]. These stable limit cycles represent Red Queen dynamics [92] where the community of one or more species continuously evolves [Fig. 3.3]. Notably, these cycles are not driven by cyclic dynamics in population size, which are not possible with purely competitive interactions and logistic growth, but by the asymmetric competition driving selection around the periodic orbit as can be seen by the selection gradient in figure 3.3.

3.3.3 Red Queen dynamics can lead to alternate levels of metastable diversity.

Notably, in simulations that result in stable limit cycles, different numbers of species may emerge [Fig. 3.4]. This emergent diversity is then maintained. Unlike an ESC, these stable limit cycles have large areas of positive invasion fitness that are reachable by small mutations – a fact that underlies the non-zero selection gradient and drives the cyclic movement. This also means that mutants can continuously invade. However, all areas of positive invasion fitness reachable by small mutations only perpetuate the oscillatory motion rather than initiating diversification.

To examine this further, we seeded the adaptive dynamics simulations with an arbitrary number of randomly chosen phenotypes (between 1 and 100 initial species). When seeded with a high number of species, most die out immediately, but many survive. Even after the system is simulated for a long period of time (100,000 branching mutations attempted), those simulations seeded with few species maintain the low diversity while simulations seeded with more tend toward higher diversity stable limit cycles or ESCs [Fig. 3.5]. For the parameterization illustrated here and a quartic carrying capacity, metastable limit cycles with 1-6, or 8 species all emerged depending on the initial diversity in the simulation [Figs. 3.4 and 3.5]. Evolutionary metastable states of 12, 13, or 14 clusters also emerged when seeded with high initial diversity. Other parameterizations of asymmetric competition (values for $b$) were also tested and while some parameterizations did not result in any cyclic
Figure 3.3: **Asymmetric competition can lead to Red Queen dynamics.** Red queen dynamics denotes a situation in which one or more populations continuously evolve on a stable limit cycle in phenotype space. Simulation were run using the radially symmetric carrying capacity and initiated with 10 random species. Panels A and B show the complete history of evolutionary dynamics, with time in panel A increasing from white to blue and carrying capacity increasing from black = 0 to white = 1. Panel C is a depiction of the population at the end of the simulation. Colors in panel C represent the invasion fitness (per capita growth rate of a new mutant if it were to arise). Positive invasion fitness is shown in shades of orange (maximum of 0.17), negative in blue, and invasion fitness equal to zero in white. Arrows are proportional to the square root of the selection gradient for each species. Simulation time was cut to only 100 time steps in the figure so the limit cycles could be more easily seen.

dynamics, alternative levels of metastable diversity were always found. Interestingly, using the quartic carrying capacity, we were unable to find a parameterization of \( b \) that resulted in a stable limit cycle at low diversity but did not eventually saturate to an ESC if seeded with a diverse initial community.

The presence of a high diversity ESS was not always the case with the radially symmetric carrying capacity. The pattern of low seeded diversity leading to low diversity metastable oscillations is the same, but high diversity stable configurations were often oscillatory as well. Many different simulations with randomly chosen asymmetric competition parameters and the radially symmetric carrying capacity seemingly had no fully saturated ESC, including the parameterization shown here [Fig. 3.4].
Figure 3.4: **Invasion fitness landscapes for alternative metastable states.** Alternative metastable states resulting from simulations with different levels of initial population diversity. Each panel represents an alternative level of metastable diversity for a single set of parameters and only differ based on the randomly generated initial communities. Points represent surviving species at the end of each simulation. Arrows are proportional to the square root of the selection gradient for each species. The surface shows the invasion fitness (per capita growth rate of a rare mutant) with positive invasion fitness displayed in orange and negative in blue. The maximum invasion fitness for each panel is displayed in the top right corner of the panel. All axes are displayed from -2 to 2. Simulations in the left two columns use the quartic carrying capacity and those in the right three columns use the radially symmetric carrying capacity. All other parameters can be found in Table B.1.
Figure 3.5: **Levels of metastable diversity.** The final evolutionary diversity when seeding the simulation with different numbers of initial species. Red indicates simulations with a quartic carrying capacity kernel, while blue are those with a radially symmetric carrying capacity kernel. Open circles are simulations with only symmetric competition. Full circles are simulations run with asymmetric competition. The $b$ values dictating the competition asymmetry can be found in Appendix B. All other parameters remained the same for all simulations and can be found in Table B.1 as well.

### 3.3.4 Large mutations push populations from lower diversity cycles toward saturated ESS

The small mutation assumption of adaptive dynamics is inflexible and necessary in order to derive the evolutionary dynamics. However, branching events are simulated manually. Therefore, we can increase the size of branching mutations (instead of a small fixed mutation $\epsilon_{\text{mut}}$, mutant phenotypes are chosen from a Gaussian distribution with mean equal to the parent and standard deviation $\sigma_{\text{mut}} \geq \epsilon_{\text{mut}}$).

With a quartic carrying capacity, when $\sigma_{\text{mut}}$ is increased to 0.05 or larger the lower diversity metastable limit cycles eventually break down and the species-packed ESS is reached (the diversity of the asymmetric ESS is 16, the same as for the symmetric case [Fig. 3.6]). This indicates that these lower diversity cycles are locally stable while the high density ESS is globally stable. For the asymmetric parameters chosen here, the saturated ESS contains 14 species [Fig. 3.4]. Of note, because branching mutations are modeled as a Gaussian distribution, even with a small $\sigma_{\text{mut}}$ transitions from lower to higher diversity limit cycles did occur, but exceedingly rarely, allowing the lower diversity meta-stable states to persist.
until the end of our simulations.

![Figure 3.6](image)

Figure 3.6: **Large mutations allow escape from low diversity meta-stable states.** The final evolutionary diversity when seeding the simulation with different numbers of initial species for differently sized mutations and asymmetric competition. For solid points, mutants were placed a small fixed distance away from the parents. For hollow triangles, mutations are drawn from a Gaussian with mean equal to the parent’s phenotype and standard deviation indicated by point color. Mutation size or standard deviation (depending on the mutation algorithm) are represented by color. All other parameters are the same as those listed in Table B.1.

For radially symmetric carrying capacity simulations without an ESS, each parameter combination seemingly has a globally stable limit cycle that is eventually reached with large enough mutations. For the parameter values used as an example in this paper, this globally stable limit cycle has 8 species on the outer ring and 5 on the inner, both which cycle clockwise. Unlike with the quartic carrying capacity, there also exist metastable limit cycles with higher diversity than the globally stable one. These “super saturated” communities also collapse to the globally stable cycle when mutation size is increased. Super-saturated stable limit cycles occurred rarely when seeded with a random initial species, but were easy to manufacture by manually placing species in trait space on approximately the two concentric circles that emerge in any community with more than six distinct species [Fig. 3.4].

Because the globally stable community undergoes non-equilibrium dynamics, there still exist areas of positive invasion fitness that drive these cycles [Fig. 3.7]. Mutants into these
areas of positive invasion fitness eventually out compete the nearby resident, returning the system to 13 species. The invasion fitness landscape around the inner ring is nearly flat, with shallow peaks, leading to nearly neutral local dynamics. This leads to the persistence of small clusters of mutants around the 5 inner species for relatively long periods of time [for a discussion on neutral coexistence see 75], explaining the high levels of diversity seen in radially symmetric simulations with large mutations ($\sigma_{mut} \geq 0.05$). Despite this apparent increased diversity, the pattern of approximately 13 species clusters is maintained long-term.

Figure 3.7: **Large mutations can cause transitions between locally stable levels of diversity.** Simulation were run using the radially symmetric carrying capacity, Gaussian distributed mutations with $\sigma_{mut} = 0.1$, and 10 initial species (randomly chosen). Panels A and B show the complete history of evolutionary dynamics, with time in panel A increasing from white to blue and carrying capacity increasing from black = 0 to white = 1. The initial population is highlighted in red. Transitions between diversity states due to rare, large mutations can be seen in the change in frequency of the limit cycles in Panel B. Panel C is a depiction of the population at the end of the simulation. Colors in panel C represent the invasion fitness. Positive invasion fitness is shown in shades of orange (with a maximum of 0.068), negative in blue, and invasion fitness equal to zero in white. Arrows are proportional to the square root of the selection gradient for each species. Dynamics of the inner circle are under weak selection and provide the environment for mutants to persist for relatively long periods of time.

### 3.3.5 Finite population sizes reduces maximal diversity and facilitates cycling

Individual-based simulations largely aligned with all the results of the adaptive dynamics [Fig. 3.8]. Because of the fully stochastic nature of the individual-based model, trajectories obviously didn’t match the adaptive dynamics exactly, but the numbers of phenotypic
clusters and direction of oscillations in those simulations with limit-cycles qualitatively aligned as expected.

![Figure 3.8](image)

**Figure 3.8: Alternative metastable states for different levels of final diversity in individual-based simulations.** Points represent individuals at the end of each simulation. The surface shows the invasion fitness (per capita growth rate of a rare mutant) with positive invasion fitness displayed in orange and negative in blue. Panels for each value of $K_{max}$ show a diversity of outcomes observed across different replicates. The maximum invasion fitness for each panel is displayed in the top right corner of the panel. All axes are displayed from -2 to 2. Simulations use a quartic carrying capacity with $K_{max} = 100$ in the left column, $K_{max} = 200$ in the middle columns, and $K_{max} = 400$ in the right. All other parameters can be found in Table B.2.
In these simulations, the overall size of the population can be regulated by a parameter $K_{\text{max}}$ that controls the height of the peak of the carrying capacity function at the origin. This does not set an artificial cap on the population and instead can be thought of as a parameter controlling the richness of the environment. When $K_{\text{max}}$ is large, there are sufficient resources available for a large population to grow. When it is small, resources are exhausted quickly and death rate increases, limiting the size of the population.

When we reduced $K_{\text{max}}$, as expected the total size of the population decreased. More interestingly, the maximum number of phenotypic clusters that emerged decreased as well. For example, with a radially symmetric carrying capacity and asymmetric competition, when $K_{\text{max}}$ was set to 400, we see 7 or 8 species emerge when starting with high initial diversity [Fig. 3.9]. However, when $K_{\text{max}} = 200$, no more than 6 species were ever maintained for a significant period of time. This was not due to demographic stochasticity, as those 6 species were often maintained in their limit cycle for very long periods of time without extinction or branching. This means that finite resources, and thus finite population sizes, limit the maximal diversity in a system, often facilitating cycling despite the presence of a theoretical global ESS.

Despite the stochasticity, the same general pattern of locally stable, low diversity limit cycles with low initial phenotypic variation and high diversity limit cycles with high initial diversity largely persists [Fig. 3.9]. However, with a very low population size [e.g., $K_{\text{max}} = 50$, Fig. 3.9], demographic stochasticity overwhelms selection maintaining the low diversity limit cycles, allowing the population to consistently transition to a more stable, higher diversity state. Nearly all replicate simulations with $K_{\text{max}} = 50$ resulted in exactly 3 stable species [Fig. 3.9]. Additionally, unlike in adaptive dynamics simulations, transitions from higher to lower diversity were also possible due to stochastic extinction [e.g., Fig. 3.10].

### 3.3.6 Small population sizes counteracts the effects of large mutations, maintaining low diversity limit cycles

With sufficiently large population sizes ($K_{\text{max}} \gtrsim 400$), increasing the size of mutations moderately had a similar effect to the adaptive dynamics simulations, allowing species to escape lower diversity limit cycles. However, larger mutations also increase the variation within species clusters. When mutation sizes were increased too much, distinct phenotypic clusters all but disappeared with individuals spread out across the entirety of the trait space. Even in these situations the population would cycle in the direction expected if a limit cycle exists.

In the adaptive dynamics, when mutations sizes increased, populations always converged on the most stable configuration, whether that be an ESS or a globally stable limit cycle. With small population size, even with increased mutation sizes, diversity levels remained low. This is because despite there being larger mutations allowing mutants to “jump” across areas of the negative invasion fitness and diversify, these new mutant species are
Figure 3.9: **Finite population reduces realized diversity.** The final number of phenotypic clusters for the individual based model when seeded with different initial population sizes. Individuals were clustered into groups by phenotypic similarity. To control for stochasticity, the final number of clusters was calculated as the median number of clusters over the last 200 time steps. Color indicates the maximum of the carrying capacity kernel (set at the origin). This represents the “richness” of the environment, with larger values modeling an environment with resources that are able to support a larger population. Simulations were run with a quartic carrying capacity kernel and all other parameters remained the same as previous simulations.

rarely able to establish. The nature of finite resources inhibiting diversification is strong enough to counteract the ability of large mutations to escape locally stable limit cycles. In these cases, while the number of species was generally maintained, there was increased demographic stochasticity, with populations diversifying and going extinct more often than with smaller mutations.

### 3.4 Discussion

We have shown here that systems based on Lotka-Volterra competition can cause many different levels of locally stable diversity emerge. This is particularly true with systems of asymmetric competition that lead to periodic evolutionary dynamics in phenotype space. These types of systems often get stuck in locally stable, low diversity limit cycles, despite the presence of a higher diversity global ESS or stable limit cycle.

Classic theory of adaptive radiations expects a quick burst of diversification, followed
by a slowdown and possible settling to an ESS – a pattern that has also been shown in natural populations [25, 64, 152, 154]. Adaptive dynamics models show these exact dynamics with successive branching until an ESS is reached [36]. This ESS does not, however, imply community saturation. As expected, our results show that in an adaptive radiation, the population will quickly diversify. If a locally stable ESS or limit cycle is reached, diversification will then come to a stop. However, with small Gaussian mutations, eventually a rare mutation may be introduced that is able to invade the population and another diversification event takes place. This latest branching event could also trigger others, until a new locally stable community is reached. This means that during the early stages of an adaptive radiation, evolution is driven by relatively quick, successive, and small mutations, leading to the expected “early burst” of diversification. However, once a locally stable state is reached, rare, large mutations are necessary to “jump” areas of negative invasion fitness and initiate further diversification, followed by another round of successive small-effect mutations. This large effect mutation mirrors the classic idea of a “key innovation” [159], opening up new areas of adaptive opportunity.

Our findings also compliment findings of non-equilibrium dynamics in higher dimensions...
By manually restraining the levels of diversity, Doebeli et al. were able to show that oscillatory and, in higher dimensions, chaotic dynamics are far more likely with lower levels of diversity. Here, we are able to generate the same non-equilibrium dynamics in two dimensions, but as an emergent property of the system. In our results, it became clear that while most systems had locally stable levels of diversity, those with non-equilibrium dynamics were particularly difficult to escape. This is because in non-equilibrium systems, mutations into areas of positive invasion fitness tend to only perpetuate the same cycle. Instead of just having to jump canyons of negative invasion fitness in order to diversify, mutants likely also have to jump across a peak or saddle point of positive invasion fitness. Given the complexity of natural systems, evolution likely takes place in high dimensions. Taken together, these two results imply that many competitive ecosystems are likely unsaturated and undergoing some form of non-equilibrium, or Red Queen, dynamics. Indeed, previous results, both theoretical and empirical, have implied that Red Queen dynamics may be more generic than previously thought and, like our system, likely stable.

Previous theory work on the evolution of diversity via competition for discrete, resources has also supported the notion that evolution often drives ecosystems to remain in an unsaturated state via a common limiting resource or a “diversification-selection balance” with substitutable resources. While these unsaturated states are maintained by different processes than the low diversity metastable states presented here, the diversity of mechanisms promoting low diversity ecosystems hints toward their possible generality in nature.

Perhaps most intriguingly, low diversity states were actually further stabilized by small population sizes. In the individual-based model, reducing the environmental carrying capacity led to smaller population sizes as expected but also a smaller number of phenotypic clusters. For a given value of $K_{\text{max}}$ there exists some approximate maximal diversity that can stably exist. This remained true even when mutation size was increased. Increasing diversity with increasing ecosystem productivity has also been confirmed empirically. In the adaptive dynamics simulations, increased mutation size allowed for mutants to jump into areas of positive invasion fitness, causing diversification. In the individual-based simulations this remained true, but these increased levels of diversity would not remain long, with one or more of the species dying out due to small population size stochasticity and increased competition. This means that in small populations, Red Queen dynamics were often perpetuated despite the presence of a higher diversity, globally stable ESS predicted by the adaptive dynamics. These non-equilibrium communities therefore remained in low diversity ESCs for perpetuity.

We should note that increased mutation size can also be considered as a proxy for migration between communities. The lack of a theoretical work on the interplay between eco-evolutionary and metacommunity dynamics is a known problem. Experimental
work measuring diversity as a function of immigration history finds that priority effects can play a significant role in shaping resulting communities [20, 49, 87, 184, 185]. As the resulting communities are shaped by historical contingencies, this supports the idea that ecosystems may have many locally stable ESSs or limit cycles. Classical metacommunity theory suggests that community similarity will increase with high rates of migration between communities and low total population sizes [21]. Both of these factors proved analogous to our results. Increased mutation size modeling migration allowed communities to escape locally stable ESCs and converge on the unique globally stable ESS or limit cycle. Decreased carrying capacity leading to reduced maximal diversity forces all communities into fewer choices of metastable diversity patterns and therefore increased community similarity.

Niehus et al. [121] propose a model in which horizontal gene transfer acts in conjunction with migration to homogenize microbial communities, suggesting an additional way for communities to escape metastable communities. While we find this idea compelling, we feel the complexity of HGT and immense diversity in microbial systems necessitate further investigation on the micro-evolutionary dynamics of HGT, representing an important and opportune area for future research.

Ultimately, the model and results presented here are broadly applicable to understanding how frequency-dependent selection can shape the realized diversity of natural communities and the dynamics of adaptive radiations. The pervasive presence of locally stable states or limit cycles in the adaptive dynamics and their further stabilization by finite population sizes suggests at their ubiquity in nature.
Chapter 4

Adaptive diversification and niche packing on rugged fitness landscapes

4.1 Introduction

The adaptive landscape has been a staple of evolutionary thinking since its introduction by Sewall Wright in 1932 [182]. These landscapes are recognized as a convenient and intuitive tool for visualizing and modelling evolutionary dynamics, despite much debate over the years [26] [178]. In particular, Wright envisioned rugged fitness landscapes, or landscapes with many local “adaptive peaks” and valleys, and stochastic shifts of a population between peaks as the model for evolutionary dynamics and speciation [13].

In Wright’s classical fitness landscape, fitness is a static quantity, immutably linked to the genotype or phenotype being modeled and based on characteristics of the given trait or environment. However, it has long been appreciated that the fitness of a given type is affected by the distribution of other types in the population [24] [109]. If fitness is in this way frequency-dependent, the fitness landscape now becomes dynamic and a function of the population present.

While the literature of rugged fitness landscapes explores the dynamics of how a single species adapts to and evolves on that landscape, attempts to explicitly describe adaptive diversification or stable coexistence of multiple types with rugged fitness landscapes remain largely absent. These models are unable to explicitly explain the maintenance of biodiversity if they do not include frequency dependence, a necessary condition for stable coexistence of different types [23].

In contrast to the rugged fitness landscape model, niche packing and coexistence theory explains the coexistence of many types in a given environment not through the presence of different adaptive peaks, but by the partitioning of a continuous phenotype space into niches [102] [143]. In these models, ecotypes are defined by a continuous phenotype that is used to calculate that type’s carrying capacity (the equilibrium population size of a monomorphic population or the frequency-independent portion of fitness). Phenotype space is then partitioned into distinct niches through frequency-dependent competitive interactions [95] [166]. Classical formulations of the carrying capacity function are unimodal
(often Gaussian) or flat. While a limited number of studies consider carrying capacity functions with multiple peaks \[34, 96, 139, 146, 148\], the effects of ruggedness in the underlying frequency-independent fitness landscape on frequency-dependent ecological dynamics and multi-species coexistence remain largely unexplored.

Here we use randomly generating rugged fitness landscapes in continuous phenotype space to explore how the emergence and maintenance of biodiversity mediated by negative frequency-dependent ecological interactions is affected by the ruggedness of the underlying fitness landscape. Ecology is described by classic Lotka-Volterra dynamics based on competition on a single, continuous phenotype axis and a simple trait substitution process is used to model evolution. Species are defined by a one-dimensional phenotype that controls both the species’ carrying capacity (the frequency-independent part of fitness) and the frequency-dependent competition. The carrying capacity function has “tunable” ruggedness (the number and steepness of local peaks can be controlled), allowing us to explore the effect of increased ruggedness on diversity. In doing so we show that while increased ruggedness does reduce the opportunities for diversification and hinder evolutionary movement in phenotype space, it has little effect on the overall diversity a system can support.

4.2 Model

4.2.1 Tunable rugged landscapes

Here we introduce a model for generating tunable rugged fitness landscapes in continuous trait space. As we consider ecological dynamics including frequency dependence, the landscapes presented here represent the carrying capacity as a function of a continuous phenotype. The carrying capacity can also be thought of as the static portion of fitness, while the frequency dependence due to competition contributes the dynamic portion of fitness that is a function of the species present in the community. The actual fitness landscape is therefore dependent on both the underlying carrying capacity landscape as well as the biological community present and can be measured as the invasion fitness (per capita growth rate of a rare mutant) landscape for any situation. Importantly, carrying capacity is defined as the equilibrium population size of a monomorphic population with a given phenotype and therefore not simply the stated fitness of an arbitrary trait, but a measurable and biologically relevant quantity.

Global carrying capacity function

The carrying capacity landscape can be separated into the underlying global carrying capacity function and the local ruggedness. While the global carrying capacity function can take any form, here we use a quartic function \( K_G(x) = \exp\left(\frac{-x^4}{4}\right) \) for a given trait \( x \). The quartic function has two main advantages. First, the unimodal curve naturally restricts
viable phenotypes to an area around the origin (approximately $[-2, 2]$ for the parameterization used here). Second, the relatively flat shape of the curve at the origin (compared to the Gaussian competition function, described below) ensures the presence of a branching point at the origin (when no ruggedness is considered) and therefore the possibility for the coexistence of multiple species [9, 36]. Additionally, using quartic carrying capacity functions avoids the pitfalls emerging from using a Gaussian carrying capacity function with Gaussian competition (see below), leading to structurally unstable continuous coexistence [62].

**Ruggedness model**

To generate the local ruggedness we take a sum of $m$ Gaussian distributions along the one-dimensional trait axis with equal spacing. The width of each Gaussian is defined by $\sigma_R$, while the height of each curve, $h_k$, is sampled from a Gaussian distribution: $h_k \sim \mathcal{N}(\mu = 0, \sigma = 1)$. From here on we will refer to $\sigma_R$ as the period of the local ruggedness. To control the amplitude of the local ruggedness and ensure that there are no negative carrying capacities, the heights are re-scaled so that the deepest “valley” in the local ruggedness has an amplitude of $A_R$. The model becomes:

$$K(x) = \left(1 + A_R \frac{R(x)}{\min (R(x))}\right) \left(1 + e^{-x^4}\right)$$  \hspace{1cm} (4.1)

$$R(x) = \sum_k h_k \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_k)^2}{2\sigma_R^2}}$$  \hspace{1cm} (4.2)

where

$$h_k \sim \mathcal{N}(\mu = 0, \sigma = 1)$$

$$x_k = x_{\min} + (x_{\max} - x_{\min}) \frac{k-1}{m-1}$$

and $x_{\min}$ and $x_{\max}$ represent the extreme range of the modelled phenotype axis.

This process results in a fitness landscape with local ruggedness that is “tunable” by two parameters: $A_R$, the amplitude of the lowest valley relative to the non-rugged carrying capacity function, and $\sigma_R$, the width of each Gaussian curve that contributes to the ruggedness. Of particular note, the number of Gaussian curves, $m$, used to generate the rugged portion of the landscape only controls the “resolution” of the ruggedness and is uncorrelated to the number of peaks in the final carrying capacity function [Fig. C.1]. For instance, for the parameters used here ($A_R \in [0, 1]$, $\sigma_R \in (0, 0.05]$), carrying capacity landscapes we generated had between 1 and 76 local peaks, despite each being created as the sum of exactly 250 ($m$) Gaussian distributions spaced equally between -2 and 2 on the one-dimensional trait axis.
A unique carrying capacity landscape is randomly generated for each simulation. For examples of landscapes generated with various values of $A_R$ and $\sigma_R$ see Figure 4.1.

### 4.2.2 Ecological dynamics

We model ecology using classic Lokta-Volterra dynamics with a single continuous phenotype $x$. All reproduction is assumed to be asexual. The population dynamics for species $i$ is defined as:

$$\frac{dN_i}{dt} = rN_i \left(1 - \sum_j \left(\frac{N_j \alpha(x_i, x_j)}{K(x_i)}\right)\right)$$

(4.3)

where $r$ is the intrinsic growth rate, $N_i$ the population size of species $i$, $x_i$ its phenotype, $K(x_i)$ its carrying capacity, and $\alpha(x_i, x_j)$ the competitive effect of species $j$ on species $i$. Here we assume competition to be Gaussian, thus the strength of the interaction between two types is symmetric and increases with their phenotypic similarity:

$$\alpha(x_i, x_j) = e^{-\frac{(x_i - x_j)^2}{2\sigma_{\alpha}^2}}$$

$\sigma_{\alpha}$ determines the width of the competition kernel. As $\sigma_{\alpha}$ decreases, the interaction strength between two different types decreases.

Ecological dynamics are thus defined by the system of ODEs ($d\vec{N}/dt$) and were numerically integrated using the Runge-Kutta-Fehlberg method. Communities are considered to have reached an ecological equilibrium when $dN_i/dt < 5 \times 10^{-8}$ for all species with a population density $N_i < 10^{-8}$ is considered extinct. All final ecological communities were confirmed to be feasible (i.e., there exists an equilibrium of all species present with strictly positive population sizes) [61] as further confirmation equilibrium was reached.

As we only consider competitive interactions (as opposed to predator-prey interactions or mutualism, etc.), all communities have a globally stable equilibrium and are therefore indifferent to initial population sizes [discussed in Chapter 2 and 71]. Likewise, as we only consider 1-dimensional phenotypes and symmetric competition, evolutionary dynamics always result in a stationary equilibrium [for discussions of non-stationary evolutionary dynamics see Chapter 3 and 39, 40].

### 4.2.3 Evolutionary dynamics

Evolutionary dynamics are modelled as a trait substitution process. Under the assumption of rare mutations, ecological dynamics are numerically integrated until equilibrium, at which point a new mutant is introduced. Species with population size less than $10^{-8}$ are considered extinct and removed. Mutants are derived from a randomly chosen parent with probability proportional to their population size and are given a phenotype sampled from a Gaussian distribution centered at the parent phenotype and with variance $\sigma_{\text{mut}}^2$ ($x_m \sim \mathcal{N}(x_p, \sigma_{\text{mut}})$). For computational ease, mutant phenotypes were re-chosen if they were closer than $\sigma_{\text{mut}}/5$ to any resident in the population as populations with very similar species can be exceedingly slow to reach equilibrium. If the mutant has a positive growth
rate in the resident population, it is added to the population and the ecological equilibrium is recalculated. Evolutionary simulations were run until 500 consecutive mutants were unable to invade, when an evolutionary equilibrium was declared. All evolutionary simulations were initiated with a single species with a randomly chosen phenotype between $-2$ and $2$.

The parameterization used here is as follows: $r = 1$, $\sigma_\alpha = 0.6$, $\sigma_{mut}^2 = 0.01$, $x \in [-2, 2]$, and $m = 250$ (the number of Gaussian curves used to generate local ruggedness). $A_R \sim [0, 1]$ and $\sigma_R^2 \sim (0, 0.05)$.

### 4.3 Results

#### 4.3.1 Saturated ecological diversity

In order to investigate how ruggedness in the carrying capacity landscape affects the expected number of species that can coexist in a given ecosystem, we conducted numerical simulation experiments saturating a given environment with an over-abundance of species (500 randomly chosen species) and allowing the community to naturally correct down to an equilibrium community. This is a simple, but classic, method of numerically calculating the ESS of a system [e.g., 28, 138, 148]. The ESS, or evolutionary stable state, of a system is defined as a community that when at ecological equilibrium is completely resistant to invasion [44]. This simulation method will inevitably slightly overestimate the ESS (e.g., of the 500 random species, none has the exact phenotype of a species in the ESS – instead, 2 species with similar phenotypes to that ESS species can coexist), but it is still a useful method to compare the diversity different systems can support. After each simulation, the invasion fitness landscape ($x \in [-2, 2]$) was calculated. All simulations concluded with less than 4% of the available phenotype space having a positive invasion fitness, verifying this algorithm in approximating the ESS diversity [Fig. C.2].

Examples of the landscapes with their final equilibrium populations can be seen in Figure 4.1.

The expected diversity of the ESS of a system with a rugged carrying capacity landscape is relatively unaffected by the period of the ruggedness ($\sigma_R$) [Fig. 4.2]. However, for very small amplitude ruggedness ($A \lesssim 0.02$) the resulting diversity is slightly higher than for completely smooth carrying capacity landscapes. For landscapes with larger amplitude ruggedness the diversity of the ESS decreases. In general, systems with low amplitude ruggedness are able to support a more diverse community than those with large amplitude ruggedness, regardless of the period of that local ruggedness.

#### 4.3.2 Adaptive diversification

To test the effect of ruggedness on diversification dynamics we placed a single randomly chosen species in systems with the same randomly generated carrying capacity landscapes
Figure 4.1: Examples of rugged carrying capacity landscapes with ESS populations. Each rugged carrying capacity landscape is shown in blue, the baseline smooth carrying capacity kernel in grey, and simulated ESS populations in red. Rows denote the amplitude of the local ruggedness ($A_R$ between 1% and 50%) and columns denote square of the period of the local ruggedness ($\sigma^2_R = 0.005$ to $\sigma^2_R = 0.05$). Local ruggedness is generated randomly for each simulation. ESS are simulated by randomly selecting 500 species with phenotype $x \in [-2, 2]$ and running ecological dynamics until equilibrium (as defined by $\frac{dx_i}{dt} < 5 \times 10^{-8} \forall i$). For pairwise invasion diagrams of the same landscapes please see Fig. [C.3]

used previously. Evolution is then allowed to proceed naturally based on the trait substitution process described above. The simulation results in an evolutionarily convergent stable community in which no small-effect mutants can invade. For example communities that result from these evolutionary simulations see Figure [C.4]

As expected for the competition kernel and carrying capacity used here, in the baseline non-rugged case, evolution always resulted the 3 species ESS [Figs. 2.1 and 4.3]. Similarly to the saturated ecological dynamics, small amplitude ruggedness in the carrying capacity landscape resulted in a slightly increased expected equilibrium diversity. For larger amplitudes ($A_R \geq 0.02$), increasing the amplitude of the local ruggedness resulted in decreased diversity at the evolutionary equilibrium. For carrying capacity landscapes with an amplitude near 1, diversification did not occur and the final population remained only the single founding species.

While the period of ruggedness ($\sigma_R$) did not affect the saturated ecological equilibrium diversity, when considering the adaptive diversification from a single species, increasing $\sigma_R$ leads to increasing diversity. For very small values of $\sigma_R$ diversification does not occur, regardless of the amplitude of the ruggedness. For landscapes with small amplitude rugged-
Figure 4.2: Ecological diversity as a function of the local ruggedness. The final diversity of ecological communities when initiated with a fully saturated initial community (500 species). The lines represent a Gaussian-weighted moving average of the final diversity for a given amplitude ($A_R$) or period ($\sigma_R$) of randomly generated local ruggedness. The shading represents the 95% confidence interval of the running mean [52]. The amplitude of the ruggedness is displayed on a log-scale. Between 250 and 500 simulations were run to generate each curve. Values of $A_R$ and $\sigma_R$ were sampled randomly from [0, 1] and (0, 0.05) respectively. The global carrying capacity is a quartic function and the strength of competition, $\sigma_\alpha = 0.6$.

ness, as $\sigma_R$ increases, the evolutionary equilibrium diversity also increases until it plateaus at a slightly higher expected diversity than the non-rugged baseline case. For landscapes with larger amplitude ruggedness, increasing $\sigma_R$ also results in increased expected evolutionary diversity, though we did not consider large enough values of $\sigma_R$ for those curves to reach a maximal level of diversity.

4.4 Discussion

Theories based on rugged fitness landscapes and frequency-dependent competition have proposed competing explanations for how diversity is generated and maintained. Rugged fitness landscape theory views local peaks as adaptive zones or available niches waiting to be filled. Evolution by natural selection (and in the asexual populations considered here) is a hill climbing process up the gradient in the fitness landscape to a local peak, at which point adaptation stalls until a stochastic “peak-shift” event, whether caused by drift in small populations [182], large-effect mutations [181], or migration [13] – or more complicated deterministic dynamics like population variance induced peak shifts [180] or environmental change causing a shift in the location of the local peaks in phenotype space, viewing rugged landscapes as dynamic seascapes [117, 159].

Theories of niche packing [Chapter 2 and 95, 102], evolutionary game theory [109], and adaptive dynamics [36, 56] imagine sympatric speciation as an adaptive radiation that is
Figure 4.3: **Evolutionary diversity as a function of the width of local ruggedness.**

The final diversity of ecological communities when initiated with a single, randomly chosen species that is then allowed to evolve. The lines represent a Gaussian-weighted moving average of the final diversity for a given amplitude ($A_R$) or period ($\sigma_R$) of randomly generated local ruggedness. The shading represents the 95% confidence interval of the running mean [52]. Of particular note, the line representing $A_R = 0$ was generated with simulations and is not simply a theoretically calculated value. All simulations with $A_R = 0$ resulted in 3 species, which is the ESS community for the non-rugged global carrying capacity function. The amplitude of the ruggedness is displayed on a log-scale. Between 250 and 500 simulations were run to generate each curve. Values of $A_R$ and $\sigma^2_R$ were sampled randomly from [0, 1] and (0, 0.05] respectively. The global carrying capacity is a quartic function with $\sigma_K = 1$ and the strength of competition, $\sigma_\alpha = 0.6$.

A natural outcome of negative frequency-dependent selection (competition) and selection for individuals to limit similarity to others in the population. These models are generally built on unimodal carrying capacity functions that represent the frequency-independent, or static, portion of fitness and act as the force of stabilizing selection. Evolutionary dynamics based on frequency-dependent competition initially resemble the same hill-climbing process until the maximum of the carrying capacity landscape is reached. While the maximum is a convergent equilibrium it may be evolutionarily unstable, i.e., prone to invasion by nearby mutants on either side, resulting in evolutionary branching. This occurs when the curvature of the competition function at this point is less than the curvature of the carrying capacity function (or in the one-dimensional case explored here $\frac{K''(x^*)}{K(x^*)} < \left| \frac{\partial^2 \alpha(x^*, y)}{\partial y} \right|_{y=x^*}$ with $x^*$ representing the phenotype of evolutionary equilibrium in question) [32, 36]. In this case, there will be disruptive selection at the peak driving the diversification of the population into multiple types. Contrary to scenarios classically imagined through rugged fitness landscape theory, now speciation does not require multiple peaks in a static fitness landscape.

By combining a rugged carrying capacity landscape with frequency-dependent competition we consolidate the intuition and expectations derived from these two bodies of theory.
We use a model of classic Lotka-Volterra ecological dynamics with frequency-dependent selection and an underlying rugged landscape for the carrying capacity function. These landscapes have tunable ruggedness, allowing us to control the average curvature and number of local peaks, while leaving the underlying global fitness landscape unchanged.

When considering both frequency-dependent selection and a rugged carrying capacity landscape, the evolutionary dynamics initially are the expected hill-climbing process. However, because selection is frequency-dependent, the actual fitness function does not strictly resemble the rugged carrying capacity landscape. If a local peak and nearby valleys are shallow, the frequency-dependent selection can “flatten” the peak in the dynamically determined fitness landscape, allowing the population to deterministically cross the valley in question and continue to evolve up the global carrying capacity gradient. Alternatively, in systems with very rugged carrying capacity functions (whether because of large $A_R$ or small $\sigma_R$), this local peak represents a convergent and evolutionarily stable equilibrium and the endpoint of any deterministic evolutionary dynamics. If the landscape has some intermediate level of ruggedness such that the local peak does represent an equilibrium but the carrying capacity is more broadly curved than the competition function at that point in phenotype space, there will exist a convergent stable but evolutionarily unstable equilibrium, i.e., a branching point, and the population will split. This pattern of diversification will continue either until the environment is saturated or adaptation stalls because of a valley in the carrying capacity function too deep for frequency dependence to flatten, or because of a local peak that is too steeply curved for diversification to occur.

As the landscape becomes more rugged, more local peaks appear in the carrying capacity function and each local peak naturally becomes smaller and with a steeper curvature. Because the stability of any equilibrium in the evolutionary dynamics is dependent on the relative curvatures of the carrying capacity and competition functions at that point, smaller local peaks represent a more stable landscape that retards diversification [Fig. 4.3]. Thus, when the carrying capacity is suitably rugged the evolutionary dynamics resemble those predicted by Wright’s shifting-balance theory. Directional selection drives the population up the carrying capacity gradient until it becomes trapped on a local peak and must then wait for a stochastic event (whether large mutation, small population mediated drift, or something else) to cross any nearby area of low fitness [for a discussion of peak-shift dynamics see 26, 96, 144]. With these rugged carrying capacity landscapes, large areas of phenotype space remain invadable but unreachable by mutations of small effect [Fig. C.2]. When considering frequency dependence these stochastic peak shifts can result in the stable maintenance of multiple types, formalizing the coexistence of many types on rugged fitness landscapes.

Unlike the evolutionary dynamics, for the ecological dynamics of fully saturated communities, the underlying global carrying capacity landscape is the greatest determinant of the level of diversity a system can support, not the nature or severity of the ruggedness
of that landscape [Fig. 4.2]. Increasing the amplitude of local ruggedness does result in a less diverse equilibrium community, though the effect is slight compared to the stark effect of ruggedness on diversification dynamics. The total number of local peaks in a landscape has little predictive power for the number of distinct types that the environment can stably support. In very rugged landscapes many of the local peaks in the carrying capacity landscape remain unoccupied and uninvasible, while in less rugged landscapes multiple types may share a single peak.

Interestingly, while increased ruggedness generally depresses diversity in a system relative to the smooth global landscape, small rugged perturbations can actually lead to an increase in community diversity. This can be clearly seen in the small amplitude diversification dynamics [Fig. 4.3] and a slight effect in the small amplitude saturated ecological equilibrium [Fig. 4.2]. This small amplitude ruggedness is not large enough to hinder any evolutionary movement of the population in phenotype space, but does add just enough variation in the carrying capacity to allow diversity to be maintained at phenotypes not included in the smooth carrying capacity ESS.

Our results affirm that suitably rugged carrying capacity landscapes generate similar diversification dynamics as predicted by peak-shift theory, but not the common narrative that the individual local peaks each represent a specific niche waiting to be filled. Increased carrying capacity ruggedness does impede evolutionary movement in phenotype space and retard diversification. However, the saturated ecosystem diversity is still largely a function of the width of the global niche space compared to the width of the competition, as predicted by niche-packing theory [36, 95], rather than the local ruggedness.
Chapter 5

Rethinking the evolution of specialization: A model for the evolution of phenotypic heterogeneity

5.1 Introduction

One of the most important and persistent topics in evolutionary ecology is the evolution of generalist versus specialists species. From a theoretical perspective, this question often takes the form of asking under what conditions will a generalist species diversify into two coexisting specialists. Given the intuitive answer that the higher the costs to being a generalist, the more evolution favours the emergence of specialization, most literature has focused on how environmental variability (both spatial and temporal) can maintain generalist strategies [1]. However, there is an oft overlooked third possibility, the emergence of phenotypic heterogeneity.

| Phenotypic heterogeneity | refers to non-heritable phenotypic variation, or individuals of a single genotype that differ in the expression of their phenotypes when in the same environment. |
| Phenotypic plasticity | refers to individuals of a single genotype that change the expression of their phenotype in response to environmental variation [51]. Using the same framework, generalists can be defined as individuals of a single genotype that all express the same phenotype consisting of the ability to perform multiple functions, while coexisting specialists refer to coexisting individuals with distinct genotypes, each only able to perform a single function. |

Table 5.1: Definitions of patterns of expression. Presented here are definitions of bacterial strategies for specialization and gene expression.

Given the emphasis on environmental variability, a majority of research proposes phenotypic heterogeneity as a bet hedging strategy, where microbial colonies can ensure that some fraction of the population is always suited for the environment, eliminating the costs
Figure 5.1: The evolution of resource specialization. Cell colour represents genotype and diamond colour indicates different resources. Generalist cells (black) are genetically and phenotypically homogeneous, and all individuals feed on both yellow and purple resources. Given a cost to this duplicative metabolism, two evolutionary outcomes are possible. Coexisting specialists (red and blue) are genetically heterogeneous, but each genotype is phenotypically homogeneous and only able to feed on a single resource. Alternatively, phenotypic heterogeneous individuals (green) are genetically homogeneous but phenotypically heterogeneous, as each individual only uses a single resource.

and time lag associated with a plastic response [8]. In addition to bet hedging in response to ecological uncertainty, phenotypic heterogeneity can exist as a form of specialization. Most examples of phenotypic specialization are asymmetrical, germ-soma (germ line-somatic) differentiation [22, 118, 163]. Other examples of phenotypic heterogeneity include altruistic division of labour [179], in which one phenotype confers an individual fitness disadvantage in order to benefit the colony as a whole, include antibiotic resistance in *Escherichia coli* [8] and *Salmonella enterica* subsp. *enterica* serovar Typhimurium, which differentiates into virulent and inflammatory phenotypes in the gut of its hosts [2, 162]. Examples of metabolic heterogeneity include nitrogen fixation and oxygenic photosynthesis in cyanobacteria [17], the metabolism of glucose and galactose in yeast [69], and the metabolism of cellbiose and glucose in *Lactococcus lactis* [160]. It has been theorized that metabolic functions like these are especially prone to persistent phenotypic heterogeneity [1].

Several mechanisms can contribute to the existence of phenotypic variation independent of environmentally driven plasticity. Examples of phenotypic dimorphisms (heterogeneity between two distinct phenotypes) have been shown to be driven by asymmetric cellular
division and stochastic state switching mediated by positive feedback loops. Stochastic gene expression is increasingly viewed as the largest contributor to phenotypic heterogeneity. Because of the relatively small numbers of molecules (mRNA, protein, and metabolic intermediates) that are required to drive many cellular processes and imperfect cellular machinery, large variations in phenotypic state are to be expected. In addition to phenotypic dimorphisms mediated by asymmetrical division and positive feedback loops, these stochastic processes can also manifest as a continuous distribution of phenotypic expression. Recent modelling efforts have helped establish the theoretical framework for the possible molecular mechanisms for maintaining phenotypic heterogeneity. In this study, we hope to understand the evolutionary processes that select for the expression of phenotypic heterogeneity, rather than the biophysical mechanisms that control it.

Recently there has been some focus on the theoretical foundation of the evolution of specialization through phenotypic heterogeneity or genetic differentiation (mutation, speciation). Each of these models examines the evolution of the expression of two competing (and possibly fully incompatible) functions. Ispolatov et al. uses this heterogeneity framework to study the evolution of multicellularity through an aggregation likelihood parameter. With the exception of Tudge et al., the remaining models track some form of the ratio of expression of two competing functions as a heritable characteristic of an individual. For instance, Sargent and Otto model the evolution of generalist versus specialist pollinator flowers via a genetically controlled attraction to pollinator species. Therefore clonal individuals will express the same strategy, indicating a genetic, rather than phenotypic, specialization. Only Tudge et al. attempts to decouple the genetic and phenotypic expression of the expression strategy. They present an individual based, game-theoretic model in which there is heritable, via asymmetric cell division, phenotypic variability with two possible phenotypes. Phenotype expression is controlled by a genetically determined probability of expression and a second genetically determined probability of “copying” a competitor’s phenotype instead of their own. In this way, the population maintains a form of quorum sensing, mandating that individuals can sense the phenotype of their encounters and probabilistically alter their phenotype accordingly. Using this model, they claim that phenotypic heterogeneity can only evolve with the presence of context-sensitive phenotype expression.

None of these models has attempted to determine when phenotypic rather than genetic heterogeneity may evolve. Ecologically, populations of generalists, coexisting specialists, and phenotypically heterogeneous individuals may all perform similarly (perhaps measured by population growth rate or the rate of resource depletion) if not be completely indistinguishable. While specialist populations are genetically polymorphic, a genetically homogeneous generalist population cannot be distinguished from a phenotypically heterogeneous population through genomics. This distinction may only be observable through modern
single cell experimental techniques, such as fluorescent microscopy or flow cytometry that examine individual levels of expression \([1]\). Given the difficulty and cost of these techniques, only recently have there been studies searching for phenotypically heterogeneous traits in bacteria. In addition to the bet-hedging based heterogeneity in *Escherichia coli* \([8]\) and *Salmonella enterica* subsp. *enterica* serovar Typhimurium \([2, 162]\) mentioned previously, phenotypic heterogeneity has been identified in the metabolism of *S. cerevisiae* \([69, 172]\), *E. coli* \([3, 122]\), and *L. lactis* \([160]\). Because of the relatively recent interest in the subject and the difficulty in distinguishing generalist and heterogeneous strategies, it is likely that phenotypic heterogeneity is more common than can be exemplified by the few cases of which we are aware.

Here, we introduce a model of phenotypic heterogeneity in microbial metabolism to determine when we can expect the evolution of phenotypic specialization (heterogeneity) and genetic specialization (speciation) from populations starting as resource generalists. By describing the population phenotype distribution of the proportional expression of competing metabolic processes as a Beta distribution, rather than the Gaussian distribution most models assume, we will be able to describe scenarios of speciation, phenotypic heterogeneity, generalists, and pure (only one resource is used) strategies. Because specialization is inherently frequency dependent, we will use an adaptive dynamics framework to model the evolution of resource competition. We will study the evolution of the mean (proportional expression of metabolic pathways) and the variance (phenotypic variability) of the phenotype distribution, in order to determine the circumstances under which different forms of phenotype expression will be favoured. We show that phenotypic heterogeneity can evolve as an alternative form of specialization even without environmental fluctuations, spatial structure, or quorum sensing previously theorized to be necessary.

### 5.2 Methods

#### 5.2.1 Model Description

We present a model of microbial growth based on the consumption of two resources, \(A\) and \(B\), governed by simple Michaelis-Menten resource kinetics. The variable \(z\) represents the fraction of energy an individual uses to consume one of two available resources (\(A\) and \(B\)) and is the value we will allow to evolve. The growth of the microbial population, \(N\), is modelled by

\[
\frac{dN}{dt} = N \left( z \frac{r_A[A]}{K_A + [A]} Y_A + g(z) \frac{r_B[B]}{K_B + [B]} Y_B - \lambda \right) \tag{5.1}
\]

where \([X]\) is the concentration of substrate \(X\), \(r_X\) is the maximum rate of consumption of \(X\), \(Y_X\) is the growth yield to the population after consumption of \(X\) (the populations increases by \(Y_X\) for every unit of resource consumed), \(K_X\) is the Michaelis-Menten constant of the consumption of \(X\) (the concentration of \(X\) at which the rate of consumption is 50%
of \( r_X \), and \( \lambda \) is the per capita death rate. The function \( g(z) \) is the resulting consumption of resource \( B \) consumption given the \( z \) consumption of \( A \) and a given constraint parameter \( c \).

\[
g(z) = (1 - z^c)^{1/c}
\]

(5.2)

When \( c = 1 \), there is a linear trade-off such that an increase in the metabolic activity of one reaction corresponds to an equivalent decrease in the other. When \( c > 1 \), there is a convex trade-off, indicating an increase in the efficacy of the consumption of one resource (\( B \)) when the individual also utilizes the other (\( A \)). The most relevant biological scenario is when \( c < 1 \), resulting in a concave trade-off. This represents partial or total incompatibility between the metabolic pathways for \( A \) and \( B \) and a decrease in metabolic activity as energetic resources are spent evenly between the two processes.

The dynamics of the substrates are modelled as:

\[
\frac{d[A]}{dt} = -N \left( z \frac{r_A[A]}{K_A + [A]} \right) + \gamma_A
\]

(5.3)

\[
\frac{d[B]}{dt} = -N \left( g(z) \frac{r_B[B]}{K_B + [B]} \right) + \gamma_B
\]

(5.4)
### Table 5.2: Parameters and variables

A description of the state variables and parameters in the model.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>microbial population abundance</td>
</tr>
<tr>
<td>$[A]$</td>
<td>concentration of substrate $A$</td>
</tr>
<tr>
<td>$[B]$</td>
<td>concentration of substrate $B$</td>
</tr>
<tr>
<td>$Y_X$</td>
<td>growth yield per unit $X$ consumed</td>
</tr>
<tr>
<td>$r_X$</td>
<td>maximum rate of consumption of substrate $X$</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>per capita death rate</td>
</tr>
<tr>
<td>$\gamma_X$</td>
<td>influx of substrate $X$</td>
</tr>
<tr>
<td>$K_X$</td>
<td>substrate concentration of $X$ when the rate of consumption is 50% of $r_X$</td>
</tr>
<tr>
<td>$\bar{z}$</td>
<td>mean of the phenotype distribution for the relative consumption of $A$, $B$</td>
</tr>
<tr>
<td>$v$</td>
<td>relative variance of the phenotype distribution</td>
</tr>
<tr>
<td>$c$</td>
<td>constraint parameter, defining the curvature of the trade-off curve</td>
</tr>
<tr>
<td>$\mu_{mut}$</td>
<td>mutation rate, fraction of mutations per birth</td>
</tr>
</tbody>
</table>

such that each substrate decreases at the rate of its consumption and is introduced back to the system at a rate $\gamma_X$.

It should be noted that any monotonically decreasing function ($g'(z) < 0$) that intersects both axes at 1 (maximal efficiency for pure strategies) can be used to model the trade-off in resource consumption. We chose the above functional form because of its ability to take both convex ($c > 1$) and concave ($c < 1$) forms and because it is symmetric around $y = x$ and $g(z) = g^{-1}(z)$. Thus, the choice of which reaction, $A$ or $B$, is associated with parameter $z$ and which is associated with $g(z)$ is inconsequential.

In order to study the evolution of phenotypic variability, instead of considering a constant phenotype $z$, we instead describe the population as a phenotypic probability distribution defined by the mean phenotype $\bar{z}$ and its variance $\sigma_z^2$. A similar method has been used to show the evolution of phenotypic heterogeneity under fluctuating environmental conditions as a bet-hedging strategy \[148\]. In order to allow for both phenotypically monomorphic (pure or homogeneous mixed strategy) and dimorphic (phenotypically heterogeneous strategy), we describe the population using a Beta distribution. The Beta distribution is a continuous probability distribution defined on the interval $[0, 1]$. It is defined by two shape parameters $\alpha$ and $\beta$.

The probability density function takes the form:

$$f(x; \alpha, \beta) = \frac{1}{\Omega(\alpha, \beta)}x^{\alpha-1}(1-x)^{\beta-1}$$  \hspace{1cm} (5.5)

$$\Omega(\alpha, \beta) = \int_0^1 u^{\alpha-1}(1-u)^{\beta-1}du$$  \hspace{1cm} (5.6)

where $\Omega(\alpha, \beta)$ represents the beta function and acts as a normalization constant to guarantee
Figure 5.3: **Beta distribution.** Each curve in (a-c) represents the phenotype distribution for a single genotype as defined by the beta distribution. Pane (d) shows the phenotype distributions for two coexisting genotypes (one in red and one in blue) and the total population phenotype distribution in dashed black.

The PDF integrates to 1. (Note, The $\Omega(\alpha, \beta)$ notation was chosen here instead of the more standard $B(\alpha, \beta)$ to help distinguish the function from resource $B$.)

The Beta distribution has the ability to be a (1) monomorphic, peaked distribution when $\alpha, \beta > 1$; (2) a monotonic, skewed distribution to either side when $\alpha > 1, \beta \leq 1$ or $\alpha \leq 1, \beta > 1$; and (3) a dimorphic U-shaped distribution when $\alpha, \beta < 1$. This makes it uniquely suitable to describe (1) generalist, (2) pure, and (3) phenotypically heterogeneous genotypes [Fig. 5.3]. Additionally, because the population variability is described via the distribution, it is unnecessary to define the mechanism of heterogeneity, whether it is stochastic gene expression, positive feedback loops, or asymmetrical cell division.

There is a one-to-one map, $(\alpha, \beta) \mapsto (\bar{z}, v)$, where $\bar{z}$ is the distribution mean and $v$ is the relative variance, or the variance of the distribution scaled so it is defined on the interval $(0, 1)$.

$$\left\{ \frac{\alpha}{\alpha + \beta}, \quad v = \frac{\sigma_z^2}{\bar{z} - \bar{z}^2} = \frac{1}{\alpha + \beta + 1} \quad \bar{z}, v \in (0, 1) \right\}$$

The $\bar{z}, v$ trait space is thus more mathematically convenient (being finite instead of infinite) and lends itself to the biologically intuitive interpretation that $\bar{z}$ and $v$ are respectively the
preference for one resource over the other and the level of variability in phenotype expression of a genotype. For the rest of the paper, we will focus on evolution in the $\bar{z}$, $v$ trait space. For a longer discussion see [D.1]

5.2.2 Equations

By integrating over the phenotype distribution we can determine the total consumption of a resource by all individuals of each genotype $i$. Based on the definition of mean $\int_0^1 zf(z;\alpha,\beta)dz = \bar{z}$, $\bar{z}$ is sufficient to describe the consumption of resource $A$. Thus, including the phenotypic distribution functions and multiple genotypes, the compete system becomes:

$$\frac{dN}{dt} = \sum_i N_i \left( \bar{z}_i \ast \frac{r_A[A]}{K_A + \langle A \rangle} Y_A + \int_0^1 g(z)f(z;\alpha_i,\beta_i)dz \ast \frac{r_B[B]}{K_B + \langle B \rangle} Y_B - \lambda \right) \quad (5.8)$$

$$\frac{d[A]}{dt} = \sum_i -N_i \left( \bar{z}_i \ast \frac{r_A[A]}{K_A + \langle A \rangle} \right) + \gamma_A \quad (5.9)$$

$$\frac{d[B]}{dt} = \sum_i -N_i \left( \int_0^1 g(z)f(z;\alpha_i,\beta_i)dz \ast \frac{r_B[B]}{K_B + \langle B \rangle} \right) + \gamma_B \quad (5.10)$$

$$\left\{ \alpha_i = \bar{z}_i \left( \frac{1}{v_i} - 1 \right), \beta_i = \frac{(v_i - 1)(\bar{z}_i - 1)}{v_i} \right\}$$

This system equilibrates for some $A^*, B^*$ for each combination of genotypes present.

We will also consider three more complicated scenarios: the inclusion of a cost to heterogeneity, cross-feeding rather than independent resource use, and a variable environment. The equations for these scenarios are included in their discussion below and the entire model including all three scenarios can be found in [D.2]

5.2.3 Evolutionary Analysis

Given the ecological dynamics given by Equations $[5.8, 5.10]$, we analyze the evolutionary dynamics using the principles of adaptive dynamics $[33, 55]$. We consider evolution in the two-dimensional $\bar{z}$, $v$ plane. To do this we calculate the invasion fitness ($f_{inv}$), defined as the per capita growth rate of a rare mutant ($\bar{z}_{mut}$, $v_{mut}$) in the environment determined by the ecological dynamics of the resident ($\bar{z}_{res}$, $v_{res}$), $A^*, B^*$.

$$f_{inv}(\bar{z}_{res}, v_{res}, \bar{z}_{mut}, v_{mut}) = \bar{z}_{mut} \ast \frac{r_A[A^*]}{K_A + \langle A^* \rangle} Y_A + \int_0^1 g(z)f(z;\alpha_{mut},\beta_{mut})dz \ast \frac{r_B[B^*]}{K_B + \langle B^* \rangle} Y_B - \lambda \quad (5.12)$$
As we are not able to solve equations \(5.8-5.10\) analytically, we must solve for the equilibrium environment of \(A^*\) and \(B^*\) numerically \([73]\). The selection gradient, \(S(\bar{z}_{\text{mut}}, v_{\text{mut}}) = (s_{\bar{z}}(\bar{z}_{\text{mut}}, v_{\text{mut}}), s_v(\bar{z}_{\text{mut}}, v_{\text{mut}}))\), is thus:

\[
\begin{align*}
  s_{\bar{z}}(\bar{z}_{\text{mut}}, v_{\text{mut}}) &= \frac{\partial f_{\text{inv}}}{\partial \bar{z}} \bigg|_{\bar{z}=\bar{z}_{\text{mut}}, v=v_{\text{mut}}} \\
  s_v(\bar{z}_{\text{mut}}, v_{\text{mut}}) &= \frac{\partial f_{\text{inv}}}{\partial v} \bigg|_{\bar{z}=\bar{z}_{\text{mut}}, v=v_{\text{mut}}} 
\end{align*}
\]

(5.13) (5.14)

Under the standard assumptions of adaptive dynamics that mutations are small and rare (equilibrium ecological dynamics are reached before a second mutation arises) and that there is a symmetric and homogeneous mutation process \([33, 55]\), the evolutionary dynamics are given by the selection gradient such that:

\[
\begin{align*}
  \frac{d\bar{z}}{dt} &= \frac{1}{2} \cdot \mu_{\text{mut}} \cdot \sigma_{\bar{z}}^2 \cdot N^*(\bar{z}, v) \cdot s_{\bar{z}}(\bar{z}_{\text{mut}}, v_{\text{mut}}) \\
  \frac{dv}{dt} &= \frac{1}{2} \cdot \mu_{\text{mut}} \cdot \sigma_v^2 \cdot N^*(\bar{z}, v) \cdot s_v(\bar{z}_{\text{mut}}, v_{\text{mut}})
\end{align*}
\]

(5.15) (5.16)

where \(\mu_{\text{mut}}\) is the mutation rate (fraction of mutations per birth); \(\sigma_{\bar{z}}^2, \sigma_v^2\) are the variances of their respective mutation distributions; and \(N^*(\bar{z}, v)\) is the equilibrium population size for the given genotype \([33]\). With this terminology, evolutionary equilibrium points, or singular points, are genotypes in the \(\bar{z}, v\) plane such that \(\frac{d\bar{z}}{dt} = \frac{dv}{dt} = 0\). In order to determine the convergence stability of the equilibrium, i.e., whether the point is an attractor, repeller, or saddle-point, we can conduct the first derivative test (calculate the sign of the real parts of the eigenvalues of the Jacobian of \(S\) evaluated at the singular point). However, convergence stability does not imply evolutionary stability or visa versa \(33\). Rather, equilibria that are convergent stable and evolutionary unstable are called “branching points” as the population will evolve to this point, then diversify into distinct lineages. Evolutionary stability, and the possibility of branching, is determined by the eigenvalues of the Hessian matrix of second derivatives of \(f_{\text{inv}}\) evaluated at the singular point. Note that evolutionary stability in a single variable can also be determined when the Hessian is evaluated at a point on the nullcline \(\frac{dx}{dt} = 0\) of another. This however, does not guarantee branching, but rather only suggests its possibility. We will revisit this point for the given model in the discussion.

Since we cannot solve for these values analytically, we must instead rely on graphical and numerical methods. To visualize evolution in a single trait, pairwise invasion plots are used. The bivariate evolutionary dynamics (simultaneous evolution in \(\bar{z}\) and \(v\)) can be visualized in two dimensions with the selection gradient \(S\). The selection gradient is calculated as the first derivative of the invasion fitness at each point \([5.13, 5.14]\). Derivatives were approximated using centred finite difference approximations with fourth-order error,
while those on the borders were approximated with one-sided finite difference approximations with second-order error \[97\]. The nullclines of each variable represent the evolutionary fixed points for that variable when the other is fixed. These nullclines were estimated as the zeros of the selection gradient in each dimension. The stability of the nullclines was also approximated using the second derivative of the selection gradient. However, the existence of a convergent stable, evolutionarily unstable nullcline does not guarantee branching. These deterministic dynamics rely on the assumptions of adaptive dynamics, namely that mutations are small and rare and that the invasion of a mutant implies its eventual fixation.

Because of the assumption that invasion implies fixation, we can only visualize the evolution of monomorphic populations. Once a monomorphic population reaches a branching line in one dimension that is not also an evolutionary stable state in the other, from the deterministic trajectories, we cannot be sure whether the population will branch or continue to evolve in the other dimension.

5.2.4 Evolutionary Simulations

In order to fully investigate the dynamics of evolution of both \( \bar{z} \) and \( v \), evolutionary simulations are necessary. Ecological dynamics are solved numerically \[73\]. New mutations are added at exponentially distributed times as a function of the population size. A parental strain \( i \) is selected to mutate proportional to its frequency in the population. The new mutant is chosen from a bivariate Gaussian distribution with mean equal to the parental evolutionary parameter values \((\bar{z}_i, v_i)\) and with a fixed variance \((\sigma_\bar{z}^2, \sigma_v^2)\). If any mutant phenotypes are infeasible (e.g., \( v_i \notin [0, 1] \)), the phenotype is chosen again from the same distribution. New mutants are added to the population at some small concentration \( N_o \) and any strains with concentration \( N_x < N_o \) are considered extinct and removed. In this way, each simulation is a trajectory of stochastic evolutionary dynamics coupled to deterministic ecological competition.

Because integrating over each phenotype distribution is computationally costly (especially with large \( v \), when the extremes of the phenotype distribution approaches vertical), we calculate a lookup table of all possible genotypes to the \( 10^{-3} \) precision. During the simulations, these integrals are calculated as the linear combination of nearest values.

Each simulation was run until it reached an evolutionary equilibrium, which we pragmatically defined as 30 consecutive deleterious mutations. A \( \bar{z} \) trajectory is considered to have branched if the weighted variance of population \( \bar{z} > 0.001 \). This cutoff was determined to roughly corresponded to the emergence of visually dimorphic populations in the two-dimensional trait space. Other cutoff values, as well as calculating the emergence of a second peak in the population phenotype distribution, were also tried, but did not qualitatively affect the results. A genotype was considered phenotypically heterogeneous if \( v > 0.98 \). Given the conservative assumption for evolutionary equilibrium, branching, phenotypic heterogeneity, and/or a pure strategy \((\bar{z} \approx 0, 1)\) was reached in every scenario.
From this we hope to determine the conditions that favour the evolution of: phenotypic heterogeneity (dimorphic phenotype distributions), homogeneous mixed and pure strategies (monomorphic phenotype distributions), and genetic specialization (evolutionary branching into two monomorphic phenotype distributions).

5.3 Results

Given a concave trade-off between phenotypes \((0 < c < 1\), indicating a partial incompatibility between pathways), there is always directional selection toward a higher \(v\) and the existence of a branching point in \(\bar{z}\). Thus, in the two-dimensional adaptive dynamics as determined by the selection gradient \(S\), there exists at least one nullcline where \(\frac{d\bar{z}}{dt} = 0\) (corresponding to the branching point in \(\bar{z}\) and from now on referred to as the “branching nullcline”) but no nullcline for \(\frac{dv}{dt} = 0\) [Fig. 5.4]. When there is a convex trade-off \((c > 1\), pathways are complementary), there is directional selection toward smaller \(v\) and the branching nullcline for \(\frac{d\bar{z}}{dt}\) becomes an attractor [Fig. D.3d]. Evolutionary singular points exist at the intersection of nullclines. Because no singular points exist (given no \(\frac{dv}{dt} = 0\) nullclines), we instead look if there exist any asymptotic trajectories in \(S\) to which the population will likely converge.

![Figure 5.4: Selection gradient. A visualization of the deterministic evolution in two dimensions for \(c = 0.3\). The \(\frac{d\bar{z}}{dt}\) nullclines are shown in blue. As there are no singular points in the one-dimensional \(v\) selection gradient, there are no \(\frac{dv}{dt}\) nullclines. Solid nullclines are evolutionarily stable in that dimension. Dashed nullclines are convergent stable but evolutionarily unstable. Dotted nullclines are unstable. \([r_A = 1.1, r_B = 1.01, Y_A = 0.8, Y_B = 0.5, \lambda = 0.01, \gamma_A = \gamma_B = 1.0, k_A = k_B = 1.0, c = 0.3]\)
5.3.1 Deterministic Evolution

When there is low compatibility between the two metabolic pathways ($c < 0.5$) and similar resources ($r_A = 1.1$, $Y_A = 0.8$, $r_A = 1.01$, $Y_A = 0.5$), there exists both an unstable and a branching nullcline in $\bar{z}$ [Fig. D.3a]. Given a small enough $\bar{z}$ and a large enough $v$ (i.e., the population does not start out as a monomorphic, resource $A$ specialist), the population will evolve along an asymptotic trajectory that somewhat follows the $\frac{d\bar{z}}{dt}$ branching nullcline. If the population does start as a phenotypically monomorphic, resource $A$ consumer, it will quickly evolve to $\bar{z} = 1$ and become a pure $A$ specialist. Depending on the initial conditions, while the evolutionary trajectory may cross a branching point, it does not strictly follow the branching nullcline.

5.3.2 Branching

Because there does not exist a singular point, branching can occur in $\bar{z}$ under two circumstances: the population branches when its evolutionary trajectory crosses the branching nullcline, or there are large enough mutations in $\bar{z}$ that “jump” from the evolutionary trajectory over the branching nullcline. In both cases, branching would occur despite continued directional selection in $v$.

When a population nears the branching nullcline we cannot analytically determine if there is stronger selection to branch in $\bar{z}$ (as would be expected if $v$ were held constant) or to continue to evolve toward higher $v$. Thus, we conducted simulations to determine the evolutionary dynamics beyond this point.

5.3.3 Evolutionary Simulations

Simulations each began similarly, with the population quickly evolving to the branching nullcline as predicted in the deterministic evolution [Fig. 5.4]. As expected, from here populations either continued along the deterministic trajectory, evolving larger $v$ and phenotypic heterogeneity or the population branches in $\bar{z}$, diverging into coexisting specialists [Fig. 5.5]. In the branching case, $v$ continues to evolve upwards until the population is fully divergent, at which point there is no longer a selection pressure on $v$ [Fig. 5.5b]. Note that because we are tracking relative variance rather than variance itself, the relative variance of a strain with $\bar{z} = 0$ or $\bar{z} = 1$ does not matter as the actual variance must equal 0 [Fig. D.1].

Because there is always selection toward larger $v$, it is possible that $\bar{z}$ branches but $v$ evolves upwards more quickly in one branch than the other, giving that branch a significant competitive advantage and driving the other branch extinct [Fig. D.5a]. This pattern of branching and subsequent extinction of one of the two branches may happen multiple times. We will refer to trajectories that branched but nevertheless result in a monomorphic population as “branching false-starts.”

Additionally, there are also cases in which $\bar{z}$ branches but $v$ fixes in one of the two
strains before the population is fully divergent [Fig. D.5b]. This results in a population that is genetically dimorphic with one pure, specialist genotype and one phenotypically heterogeneous one.

![Figure 5.5: Evolutionary trajectories. Examples of the simulated trajectories of $\bar{z}$ and $v$ showing a phenotypically heterogeneous population (a) and a genetically dimorphic one (b). Blue represents the genetic values of $\bar{z}$ and red represents the values of $v$. The size of the dots indicates the relative population size of that genotype. The y-axis is time measured by the number of mutations. Because we show both variables on the same axis, we are showing a 2-dimensional projection of the 3-dimensional space. All simulations are run with the same parameterization and run until evolutionary equilibrium, which is defined as 30 consecutive unsuccessful mutations. $r_A = 1.1, r_B = 1.01, Y_A = 0.8, Y_B = 0.5, \lambda = 0.01, \gamma_A = \gamma_B = 1.0, k_A = k_B = 1.0, c = 0.3, \bar{z} = 0.3, v = 0.1, \mu_{mut} = 1^{-5}, \sigma^2_{\bar{z}} = \sigma^2_v = 0.02$]

5.3.4 Mutation Size

As the size of $\bar{z}$ mutations decreases relative to $v$ mutations ($\bar{z}$ mutations are drawn from a Gaussian distribution with a smaller variance), the probability of phenotypic heterogeneity increases [Fig. 5.6]. Moreover, as the size of all mutations decreases ($\sigma^2_{\bar{z}} = \sigma^2_v$), the probability of phenotypic heterogeneity increases as well. In this base parameterization, the chance of populations that are both phenotypically heterogeneous and genetically dimorphic, is small (at most 5% of trajectories for any mutation size), and thus the probability of branching and the evolution of the evolution of coexisting specialists is roughly the inverse of Figure 5.6.

5.3.5 Cost to Heterogeneity

While we are most interested in the costs involved with simultaneous expression of two metabolic pathways, one could also imagine the existence of a cost of the maintenance
Figure 5.6: **Probability of phenotypic heterogeneity as a function of mutation size.** Trajectories that result in a phenotypically heterogeneous population for $\bar{z}$ are shown with solid lines. Dashed lines indicate the probability of branching false-starts for the same parameterization. The dotted line represents simulations where $\sigma_v^2 = \sigma_{\bar{z}}^2$. Branching false-starts are not shown for $\sigma_v^2 = \sigma_{\bar{z}}^2$.

$\begin{align*}
\mathbb{P}(\bar{z}) &= \frac{r_A A}{K_A + A} Y_A + \int_0^1 g(z; \alpha_i, \beta_i) dz + \frac{r_B B}{K_B + B} Y_B - \lambda
\end{align*}
$(5.17)

With this added cost, there is no longer simple directional selection for higher $v$. This can be visualized as the appearance of an attracting $\frac{dv}{dt} = 0$ nullcline and a convergent stable, evolutionary unstable singular point in the two-dimensional adaptive dynamics when $c_v > 0.55$ for our base parameterization [Figs. 5.7, D.4]. Unsurprisingly, adding a cost to heterogeneity greatly decreases the probability of phenotypic heterogeneity. When $c_v$ is large enough such that the singular point does exist, branching in $\bar{z}$ is essentially guaranteed. This is because when the population converges to the singular point, $v$ is no longer invasible and thus the system can be reduced to evolution in a single variable ($\bar{z}$) that is under disruptive selection. Even when $c_v$ is small, such that there is no singular point, the probability for phenotypic heterogeneity is still greatly decreased [Fig. D.7]. The added cost reduces the strength of selection for higher $v$ but does not affect the selection pressure on $\bar{z}$, favouring evolutionary branching.

**5.3.6 Unequal Resources**

Up to this point we have only considered relatively equal resources ($r_A = 1.1$, $r_B = 1.01$, $Y_A = 0.8$, $Y_B = 0.5$). Because of this, branching often occurs relatively symmetrically, where
Figure 5.7: Cost to heterogeneity. The selection gradient when there is a cost added to being heterogeneous ($c_0 = 0.7$). The $\frac{dz}{dt}$ nullclines are shown in blue and the $\frac{dv}{dt}$ nullclines are shown in red. Solid nullclines are evolutionarily stable in that dimension. Dashed nullclines are convergent stable but evolutionarily unstable. Dotted nullclines are unstable. There exist two singular points, one unstable and one convergent stable and evolutionarily unstable. The jagged sections of the nullclines are approximation errors due to sections of the selection gradient being very close to 0. $[\lambda = 0.01, \gamma_A = \gamma_B = 1.0, \kappa_A = \kappa_B = 1.0, c = 0.3, \bar{z} = 0.3, v = 0.1, \mu_{\text{mut}} = 1^{-5}]$

the two branches evolve at similar rates [e.g., Fig. 5.5b], and populations that evolve to be both genetically polymorphic and phenotypically heterogeneous are very rare. However, when the resources are uneven, this is no longer the case, as selection toward one resource dominates. Here, situations arise where one strain evolves as a specialist on the dominant resource and the other evolves to be phenotypic heterogeneous, supplementing its diet of the dominant resource with the poorer one [Fig. 5.8]. Because the model is written so that the cost to maintain a dual metabolism is not symmetric, but falls on the metabolism of resource $B$ ($g(z)$ modifies the uptake of resource $B$, see Equation 5.4), when resource $B$ has a higher yield than $A$ ($Y_B > 0.8$), branching most likely occurs, while when resource $A$ has the higher yield, phenotypic heterogeneity is more common.

5.3.7 Cross-feeding

As a different method of unbalancing the resources we also consider a cross-feeding scenario, in which the byproducts of the metabolism of $A$ are substrate $B$. Previous theoretical work has shown that genetic polymorphisms can evolve given such cross-feeding resource dynamics [35]. The equation for the dynamics of resource $B$ becomes:

$$
\frac{d[B]}{dt} = \sum_i N_i \left( Y_{cf} \bar{z}_i \frac{r_A[A]}{K_A + [A]} - \int_0^1 g(z)f(z; \alpha_i, \beta_i) dz \frac{r_B[B]}{K_B + [B]} \right) + \gamma_B
$$

(5.18)
Figure 5.8: **Phenotypic heterogeneity with unequal resources.** Trajectories that result in a genetically dimorphic population for $\bar{z}$ are shown in blue; phenotypic heterogeneous populations in blue; populations with both phenotypic heterogeneous and pure specialists are in purple; and genetically monomorphic, pure strategy populations in green. $[r_A = 1.1, \quad r_B = 1.01, \quad Y_A = 0.8, \quad Y_B = 0.5, \quad \lambda = 0.01, \quad \gamma_A = \gamma_B = 1.0, \quad k_A = k_B = 1.0, \quad c = 0.3, \quad \bar{z} = 0.3, \quad v = 0.1, \quad \mu_{\text{mut}} = 1^{-5}, \quad \sigma_B^2 = \sigma_A^2]$}

where $Y_{cf}$ is the stoichiometric cross-feeding yield, i.e., how much of resource $B$ is created for the metabolism of each resource $A$. Cross-feeding simulations were done with $\gamma_B = 0$ so that all of resource $B$ in the environment is created as a byproduct of $A$ metabolism.

When $Y_{cf} = 1$, the evolutionary dynamics of cross-feeding scenarios did not differ significantly from those with unconnected resource pathways. Visually, the selection gradient is qualitatively the same as those with parallel rather than hierarchical pathways [Data not shown]. Cross-feeding scenarios show a qualitatively similar propensity to branch as those with parallel resource use [Fig. D.6]. As cross feeding was not the main goal of this paper, these patterns were not investigated further.

### 5.3.8 Variable Environment

The classical theory for the evolution of phenotypic heterogeneity predicts that greater heterogeneity (plasticity) will evolve as a bet hedging strategy in variable environments, a theory that has seen significant theoretical support [54, 72, 148, 150]. Given the already significant theoretical work on the evolution of plasticity in variable environments, this was not the emphasis of our work. Nevertheless, in order to test the model and this hypothesis, we modelled resource influx as a periodic function defined by a period ($T_X \in (0, \infty)$), amplitude ($\omega_X \in [0, 1]$), and mean influx rate ($\gamma_X$) such that

$$\frac{d[A]}{dt} = \sum_i -N_i \left( \bar{z}_i * \frac{r_A[A]}{K_A + [A]} \right) + \gamma_A \left( \omega_A \sin \left( \frac{2\pi}{T_A} \right) + 1 \right)$$

(5.19)
Figure 5.9: Phenotypic heterogeneity in a variable environment. Trajectories that result in a phenotypically heterogeneous population for $\bar{z}$ are shown with solid lines. Dashed lines indicate the probability of branching false-starts for the same parameterization. The solid blue point represents the probability of branching in a stable environment ($\omega_A = \omega_B = 0$) and the blue open point represents the corresponding false starts. $[r_B = 1.01, Y_A = 0.8, Y_B = 0.5, \lambda = 0.01, \gamma_A = \gamma_B = 1.0, k_A = k_B = 1.0, c = 0.3, \bar{z} = 0.3, v = 0.1, \mu_{mut} = 1^{-5}, \sigma_\bar{z}^2 = 0.02, \omega_A = 1, \omega_B = -1]\$

\[
\frac{dB}{dt} = \sum_i -N_i \left( \int_0^1 g(z) f(z; \alpha_i, \beta_i) dz \ast \frac{r_B[B]}{K_B + |B|} \right) + \gamma_B \left( \omega_B \sin \left( \frac{2\pi}{T_B} \right) + 1 \right) \quad (5.20)
\]

Here we only considered out of phase, periodic resource fluctuations ($\omega_A = -\omega_B = 1$). In accordance with existing theory, the probability of the evolution of phenotypic heterogeneity, rather than genetic diversification, increases in a variable environment [Fig. 5.9]. When environmental fluctuations are very fast, the resource concentration in the environment mimics a constant environment and the probability of phenotypic heterogeneity is thus approximately equivalent to scenarios with constant resource influx. However, as the fluctuations become slower, individuals only able to metabolize one resource die when that resource is not available, strongly favouring the evolution of phenotypic heterogeneity over branching. If the fluctuations are slowed even further relative to the rate of evolution, such that only one of the resources is available for a sufficiently long time, that resource specialist will likely fix in the population before the next resource become available.

5.4 Discussion

There has been a recent increase in focus on the ecological consequences and evolution of phenotypic heterogeneity in microbial populations. Historically, a majority of this focus has been on phenotypic plasticity, the phenotypic response to changing environmental conditions [72, 148, 177], or heterogeneity as a bet-hedging strategy [132, 174]. This focus on
plasticity is understandable given the obvious biological and evolutionary relevance (e.g., evolution of antibiotic resistance and in response to environmental change). However, both of these explanations require environmental variation as the underlying cause of phenotypic heterogeneity. Yet it is also clear that even in controlled conditions with minimal environmental variation, there can exist large phenotypic variation between cells of the same genotype [45, 168]. In addition to dealing with fluctuating and/or extreme environmental conditions, this standing phenotypic variation has been theorized to be a mechanism of specialization [1, 67, 69, 85] and perhaps the precursor to the evolution of multicellularity [80].

Importantly, this variation can be regulated by the cell [116, 128, 140]. This regulation allows for selection on the phenotypic variation [130, 141, 167], a process that has been observed experimentally both in response to a fluctuating environment [14, 120] and in the presence of competing resources as a form of specialization [3, 69, 122]. Current theoretical work that predicts the evolution of phenotypic heterogeneity [115, 145, 148, 183] does so with the same basic condition as the prediction for sympatric speciation [37, 80, 85], namely the presence of a concave trade-off between two phenotypes. What is conspicuously absent from the existing literature is a formulation of the conditions that favour genetic versus phenotypic differentiation.

Here we considered a model capable of describing the evolution of both genetic and phenotypic variation in microbial populations. The aim of the work was to use a simple model of evolution of microbial metabolism that provides an alternative to genetic specialization and introduce a theoretical framework that can describe three types of multiple resource use: generalists, coexisting specialists, and phenotypic heterogeneity.

Despite the existence of a branching nullcline in the resource preference $\tilde{z}$, branching is often inhibited by persistent directional selection for increased phenotypic variance $v$. Branching only occurs given large mutations that facilitate mutational “jumps” across the branching nullcline, or given a cost to larger variance that decreases the strength of selection on $v$. Thus the evolutionary dominance of phenotypic heterogeneity is due to two main causes: the curvature of the fitness landscape compared to the size of mutation, and the location of the branching nullcline in the two dimensional trait space.

As mentioned previously, the evolutionary stability of a singular point is determined by the Hessian of second derivatives of the invasion fitness function. Thus the strength of selection at a branching point is determined by these second derivatives. This is in contrast to the strength of directional selection, which is determined by the selection gradient $\mathbf{S}(\tilde{z}_{mut}, v_{mut})$. A population located on the $\frac{d}{dt}$ nullcline corresponding to a branching point in $\tilde{z}$ is therefore being acted on by both first-order directional selection toward larger $v$ and the second-order disruptive selection of $\tilde{z}$, in which the continued success of either selection process suppresses the selection on the other. Ito and Dieckmann recently developed an elegant analytical treatment of evolutionary branching in bivariate trait spaces.
They showed that, given directional selection in one trait and disruptive selection in another, branching only occurs if mutations in the trait under disruptive section and/or the strength of disruptive selection are large enough compared to the mutation size and strength of directional selection in the other trait [83, 84]. The model we present here is a specific example of this directional selection in one dimension (\(v\)) suppressing disruptive selection in another (\(\bar{z}\)). However, here the relative strengths of selection in each direction are intrinsically coupled, because increasing the selection on one variable also increases the selection on the other (i.e., smaller \(c\) leads to a steeper slope in the \(v\) direction of the fitness landscape as well as a sharper curvature in the \(\bar{z}\) direction). However, in accordance with [83, 84] we find that the evolutionary outcome of directional versus disruptive selection depends on the relative size of mutations in each dimension [Fig. 5.6], with smaller mutations in the trait under disruptive selection favouring the evolution of phenotypic heterogeneity.

Of course, the conditions for branching are most relevant when the population is actually at a branching point. In this vein, it has been shown that increasing the number of evolving traits increases the probability of disruptive selection (branching) in one of them [38, 43, 165]. However, Svardal et al. point out that the increased dimensionality of the trait space will also increase the probability that a branching point will cease to be a singular point in the higher dimension (or becomes a saddle point), diminishing the effect of disruptive selection [165] (see Chapter 3 for a larger discussion on high dimensional, non-equilibrium dynamics). Indeed, this is the exact scenario presented here. The branching point that can lead to sympatric speciation for resource specialists [e.g., 37, 85] is no longer a singular point when considering the evolution of phenotypic variance as well.

The second factor leading to the dominant evolution of phenotypic heterogeneity concerns the location of the asymptotic evolutionary trajectory in the \(\bar{z}, v\) trait space [Fig. D.3a]. When \(c\) is small, like the \(c = 0.3\) scenarios we ran for our base evolutionary simulations, the asymptote is near, but not on top of, the \(\frac{dz}{dt}\) nullcline corresponding to the branching point. Given a small initial relative variance (initial population is monomorphic), the population will evolve toward the asymptote, perhaps crossing the evolutionary branching line. When the trajectory does reach the branching line, branching in \(\bar{z}\) is under second-order selection while directional selection on \(v\) is a first-order process. Thus, in most cases the population will not branch, instead it will continue to evolve in \(v\) toward the asymptote. As the population tracks along the asymptote, branching must be initiated by a mutation in \(\bar{z}\) to the opposite side of the branching line. Such a mutation would create a genetically dimorphic population with \(\bar{z}\) genotypes on either side of the branching line, possibly leading to continued diversification (barring the dominant evolution of \(v\)). However, because there is a gap in the trait space between the asymptote and nullcline, a fairly large mutation is required to initiate this branching process. Like before, this also relates to the size of possible mutations (\(\sigma^2\)) [Fig. D.5b]. As the mutation size increases, \(\bar{z}\) mutations are increasingly likely to “jump” the \(\frac{dz}{dt}\) nullcline, perhaps even before the population reaches the branching
point, initiating branching and diminishing the strength of selection on $v$.

Additionally, while decreasing the curvature of the trade-off curve ($c$ is increased toward 1) does affect the strength of selection on both $\bar{z}$ and $v$, it also moves the evolutionary asymptote closer to the branching line [Fig. D.3], increasing the probability of branching. Moreover, decreasing the strength of selection also decreases the rate at which maladapted genotypes persist in the environment. This results in a much wider cloud of persistent individuals in the trait space, increasing the probability of persistent residents and/or new mutants appearing on both sides of the branching line and initiating the branching process. Reciprocally, even slightly maladapted individuals under strong selection will die quickly, necessitating a single, large $\bar{z}$ mutation to initiate branching. Thus, populations with weak selection, or small mutations, are much more likely to branch, while populations under stronger selection or larger mutations are more likely to evolve to be phenotypically heterogeneous.

In the presence of a cost to phenotypic variance, if the cost is high enough ($c_v > 0.55$) there exists an attractor in $v < 1$ [Fig. D.4]. The presence of this attractor means there is now a convergent stable, evolutionary unstable singular point in $(\bar{z}, v)$-space, rather than just a branching nullcline for $\bar{z}$. In general, evolutionary branching in phenotype spaces with dimensions larger than 1 is an interesting and non-trivial problem [57]. In the present case of a 2-dimensional phenotype space, once the singular point is reached, the system can effectively be reduced to one-dimensional evolution in $\bar{z}$ with a fixed $v_r$. As a branching point exists in $\bar{z}$ for all $v < 1$ [Fig. D.2], branching may be delayed but is eventually guaranteed. Thus, given a high enough cost to heterogeneity, genetic specialization is always obtained. However, even when this cost is small, such that there does not exist a a singular point for $v$ [Fig. D.4], the probability of phenotypic heterogeneity is greatly decreased [Fig. D.7]. This is because the added cost to heterogeneity reduces the strength of selection on $v$ (the slope of the fitness landscape along the $v$ axis), while leaving the strength of disruptive selection in $\bar{z}$ (curvature of the fitness landscape) unchanged. This changes the speed of evolution, slowing down evolution in $v$ and returning us to the branching conditions stipulated by Ito and Dieckmann [83, 84].

Here, we have used a model of microbial metabolism for two resources and an adaptive dynamics framework to investigate the evolution of genetic versus phenotypic differential resource usage. It is clear that given large mutations or a small cost to high phenotypic variation, populations will likely diverge, while in most other cases the evolution of phenotypic heterogeneity is dominant. Moreover, when the two resources are unequal, divergence into one specialist and one phenotypically heterogeneous generalist is also possible [Figs. 5.8, D.6], a phenomenon that has already been observed in $L. lactis$ [160] and $S. cerevisiae$ [172].

Most of the existing theoretical literature concludes that a variable or structured environment is necessary for the evolution of phenotypic heterogeneity or does not consider
While we do confirm that environmental variability does help drive the evolution of phenotypic heterogeneity, it is far from a necessary, nor even a sufficient condition. Rather, our results show that phenotypic heterogeneity can evolve as a form of specialization even in a stable, homogeneous environment. However, making specific predictions as to when we should expect phenotypically rather than genetically heterogeneous populations is difficult as it depends on the size of the effect of relevant mutations. There is some indication that mutations in bacteria occur often with small effect [131], a fact that could suggest high rates of phenotypic heterogeneity in bacteria. Recent advances in experimental approaches have yielded multiple examples of phenotypic heterogeneity of metabolic traits in laboratory environments [69, 160, 172], but investigations in natural environments remains difficult given the complication of measuring both phenotypic and genetic variation simultaneously [1, 186]. Nonetheless, in addition to the examples of phenotypic heterogeneity described in laboratory conditions, we show theoretically that phenotypic heterogeneity can evolve as an alternative form of specialization, suggesting that phenotypic heterogeneity may play an important role in microbial community function in natural environments.
Chapter 6

Conclusion

In this thesis I have presented four chapters, each modelling a question related to the evolution and maintenance of diversity on both ecological and evolutionary timescales. In Chapters 2, 4 I present a model based on the classical Lotka-Volterra ecological dynamics with competition and carrying capacity defined by a phenotype in one or more dimensions. The model used in Chapter 5 is instead based on ecological growth derived from explicit resource dynamics. All four chapters also consider the evolutionary dynamics of these systems. In Chapters 2, 3, and 5 these dynamics are modelled using the framework of adaptive dynamics. In Chapter 3 in addition to the standard ODE-based adaptive dynamics, I also consider a stochastic, individual-based implementation and an implementation using PDEs. For Chapter 4 evolutionary dynamics are modelled using simpler “ecology plus mutations” simulations, but based on similar assumptions of small and rare mutations to adaptive dynamics.

6.1 Chapter specific conclusions

6.1.1 Chapter 2

In Chapter 2 I compare the diversity both generated and maintained on ecological timescales through a random community assembly process to the diversity of the ESS, or the theoretical endpoint of evolutionary dynamics. Classical theories of niche-packing all examine the diversity of the ESS, or when the community is fully saturated. However, there is considerable debate over whether real-world biological communities are saturated (at an ESS) [107].

By comparing the diversity of randomly assembled communities (a classic and well accepted theoretical method for studying community diversity [108]) I am able to show that, given a diverse enough founding population, these communities will always have diversity exceeding that of the diversity of the ESS (i.e., they are super-saturated). Perhaps most interesting, despite the diversity of the ESS increasing exponentially with dimension, the maximal diversity of the randomly assembled communities always approaches approximately 2-3 times the ESS diversity, regardless of the dimension. While incredibly dense and super-saturated communities are easy to manufacture artificially, they are almost never generated during random community assembly, putting a cap on the realizable diversity in a given system. Moreover, randomly assembling saturated or super-saturated communities
through random assembly is increasingly difficult as dimension increases. When competition takes place across a high-dimensional phenotype space, even though a saturated community is theoretically possible to assemble, the diversity of the founding population quickly increases beyond what is likely, or even possible, to occur in nature.

Additionally, I assembled communities through both top-down assembly (entire founding population is introduced at once) and bottom-up assembly (species are introduced sequentially and the community is allowed to equilibrate between species introductions). Communities assembled through the bottom-up assembly process resulted in a slightly less diverse community than those assembled from the top down. However, this difference was minor and both communities assembled through both processes generate the same basic results. This is reassuring, as top-down and bottom-up processes are the logical extremes in random assembly processes, so any natural community will likely fall somewhere in between (not all species introduced at the same time, but equilibrium not always being reached before the next species invades), confirming the applicability of this result to more complex and realistic assembly processes.

6.1.2 Chapter 3

In Chapter 3 I extend the same model to consider asymmetric competition in a 2-dimensional trait space. In doing so I am able to show that when evolutionary dynamics are limited to small-effect mutations, systems that exhibit cyclic evolutionary dynamics can often get stuck in low-diversity alternative metastable states. In these states, the asymmetry in the competition function pressures species to continually evolve (a situation previously named the Red Queen hypothesis [173]). When this is the case, any mutation of small phenotypic effect either is deleterious in the context of the current community or perpetuates the cyclic dynamics. Most importantly, the cyclic dynamics are not unique to a specific community or level of diversity. Depending on the specific species in the founding population, many different communities can evolve in systems that are otherwise identical. These differing communities are then maintained in perpetuity. Even when large mutations are considered as well, many of the metastable states are fairly stable. The specific mutation needed to break out of the given configuration can be very rare, and the communities will remain in the that metastable state for relatively long periods of time.

Importantly, these metastable states do not only occur for systems with cyclic evolutionary dynamics, but the cyclic dynamics make them more common. In one example described in the chapter, low diversity metastable states show cyclic Red Queen dynamics, but higher diversity metastable states are stable (selective pressures hold species’ phenotypes constant). In this case, both metastable limit cycles and metastable states can occur in the same system depending on the number of species present. When the community is in a metastable configuration (that is not the ESS), all small-effect mutations are deleterious in the context of that community and only very specific, large-effect mutations are able to
invade.

Interestingly, small-effect mutations are not the only mechanisms that force communities into low diversity communities. By instead modelling the system using an individual-based model with a finite population size, we are able to control the approximate carrying capacity of the community. In resource poor environments (when the environment can only support a small number of individuals), the resulting community is also less diverse. Rather than being subdivided into many small species, the community is more likely to divide into a smaller number of comparatively larger species groups. Thus, in natural populations with finite population sizes, both the finite population and the rarity of large-effect mutations are likely restricting the evolution of diverse communities.

In Chapter 2, I describe how in higher dimensions the random assembly of saturated communities is prohibitively hard. However, in that chapter I only consider symmetric competition, so if evolution is considered the community will always evolve to the ESS, regardless of the initial ecological community. However, while not tested, there is no reason to believe that community assembly with asymmetric competition is any more likely to generate saturated or super-saturated communities. Taken with the results from Chapter 3 this indicates that both community assembly and non-stationary evolutionary dynamics often trap communities in lower diversity states, suggesting the possible ubiquity of unsaturated communities in the natural world.

6.1.3 Chapter 4

In Chapters 2 and 3, I use ecological and evolutionary dynamics based on the theories of niche-packing, negative frequency dependence, and limiting similarity to model diversity. However, Sewall Wright’s rugged fitness landscapes are perhaps the most classical and iconic metaphors to explain diversity. In Chapter 4 I synthesize these two classical theories and create a model that includes both frequency dependent competition and a rugged carrying capacity function (the frequency independent part of fitness). In doing so, I am able to compare the two general views on how diversity is maintained.

In the classical theory of rugged fitness landscapes, evolution drives the population up the fitness landscape in an optimization process to a local peak. Evolution then halts there until a stochastic “peak-shift” event (e.g., small population induced drift or a large effect mutation) allows the population to cross the intervening area of low fitness to the next peak. In this modelling framework stable coexistence is not possible, though it is often assumed that each local peak represents a niche that a species can inhabit. In contrast, in the niche-packing framework (as used in Chapters 2 and 3), frequency-dependent selection drives species to “limit their similarity” and naturally subdivide the continuous niche space (most often assumed to be monomorphic) into distinct species.

When, in Chapter 4 I consider both rugged fitness landscapes and frequency dependent selection in a single model, I show that both of these theories provide an intuition for certain
scenarios. When the carrying capacity landscape is sufficiently rugged, opportunities for diversification are limited and evolutionary dynamics resemble the local optimization and stochastic peak-shift dynamics predicted by Wright’s original theory. However, the degree of the ruggedness of the landscape (measured in the approximate height and number of the local peaks) has little effect on the number of species the system can support. Instead, the maximal diversity of a system is largely determined by the relative width of the competition function to the global carrying capacity function, not the local ruggedness, as predicted by niche-packing theory.

6.1.4 Chapter 5

In Chapter 5 I consider the evolution of phenotypic heterogeneity, or when genetically identical individuals express different phenotypes. While this chapter is a topical deviation from the previous three as I am not explicitly investigating the expected diversity of a community, it largely considers the same theme. Here, instead of assuming a one-to-one map between genotype and phenotype, I recognize that variation in a population can be generated by both genotypic (i.e., diversification) and phenotypic (i.e., heterogeneity) mechanisms. With that appreciation, in Chapter 5 I create a model that allows for the same trait (in this case the relative utilization of two resources) to be expressed both genetically and phenotypically. I do this by modelling the evolution of two traits, the mean and variance of a distribution (Beta distribution) that can be either monomorphic or dimorphic depending on the values of the mean and variance. In doing so I am able to simply model generalists (individuals that utilize both resources), specialists (individuals that specialize on only one resource), and varying degrees of phenotypically heterogeneous individuals that switch between specializing on the two resources.

When set with a cost to being a generalist (a common assumption), there exists disruptive selection for the population to diversify into coexisting specialists and a directional selection toward phenotypic heterogeneity. In the stable environment modelled here, a population of coexisting specialists and a population of phenotypically heterogeneous individuals can be phenotypically identical, leading to an evolutionary race between diversification and the evolution of phenotypic heterogeneity. However, because diversification is a second-order process (i.e., diversification depends on the second derivative of the selection gradient) and the directional selection towards phenotypically heterogeneity is a first-order process, phenotypic heterogeneity is the more likely outcome. Interestingly, if we consider large-effect mutations, these mutations are more likely to drive the population towards genetic diversification than heterogeneity. This is because large-effect mutations have the possibility of “jumping” the branching nullcline (the line in the 2-dimensional phase space that represents a fitness minimum and therefore the phenotypes at which evolutionary branching will occur), kick-starting the diversification process.
6.2 Future directions

6.2.1 High dimensional competition

While I feel the results presented here tell an intriguing story about the interaction between abiotic and biotic (specifically competition) in driving the assembly of diverse communities, there remains much yet unexplored. Perhaps most significant, there is very good reason to believe that biological interactions are both asymmetric \cite{92} and take place in high dimensions \cite{39, 40}. When asymmetric competition is considered in higher dimensional trait spaces, evolutionary dynamics are more likely to be non-stationary and in dimensions greater than 2, chaotic \cite{39}.

While in Chapter 2 I consider up to 5-dimensional trait spaces, I only consider symmetric competition to ensure the presence of an ESS, which allows for the comparison of stable diversity between ecological and evolutionary timescales. Extending this study to consider asymmetric competition in higher dimensions would therefore require a new methodology to deal with cyclic and chaotic evolutionary dynamics but is definitely intriguing. In Chapter 3 I show how even in 2-dimensional trait spaces, cyclic evolutionary dynamics can trap populations in lower diversity metastable states. Considering systems with these alternative metastable states in addition to simpler ESSs offers the possibility of a more nuanced (yet complex) way to compare diversity between ecological and evolutionary timescales.

Chapters 3 and 5 both consider a 2-dimensional trait space. In Chapter 5 this is because the traits considered are specified and describe the mean and variance of a resource utilization distribution, so further extensions into higher dimensions are unnecessary. However, for Chapter 3 I limited the trait space to 2-dimensions as the goal of the study was to provide a case study and proof of concept for how cyclic evolutionary dynamics can result in alternative metastable states. A large-scale investigation of the dynamics in higher dimensions would have been an unnecessary complication. That being said, based on the works I have done, I do not have an intuition on if metastable states are also possible for systems with high dimensional competition and chaotic evolutionary dynamics, which I find worthy of future study.

Chapter 4 examines adaptive diversification and community assembly dynamics on only 1-dimensional rugged carrying capacity landscapes. Over the course of working on this project I wrote the model using different methods of generating landscape ruggedness that were not presented here, including periodic ruggedness (which resulted in unnatural resonances between the frequency of the periodicity and the width of the competition function), random ruggedness derived from Fourier transformations of Gaussian distributed noise (which resulted in a practically identical landscape to the method presented here, yet technically more complicated), and higher-dimensional carrying capacity landscapes. Considering higher dimensional landscapes seemed particularly relevant for this project, as the ruggedness of high-dimensional trait spaces has been the focus of both significant
study and controversy [53, 117, 127]. However, I realized that for the result I found most important, that the evolutionary dynamics are certainly affected by landscape ruggedness but the maximal ecological diversity of a community is not, using a 1-dimensional trait space was sufficient. Considering higher-dimensional trait spaces had no bearing on the result. However, given how integral high-dimensional trait spaces are to the conversation and debate surrounding the evolutionary dynamics on rugged fitness landscapes, I feel that further investigation would be fruitful. The model I presented here is unique in being able to describe adaptive diversification and evolution dynamics on these rugged fitness landscapes. Investigating how landscape ruggedness affects the probability of cyclic or chaotic dynamics would be both novel and relevant to both the adaptive dynamics and rugged fitness landscape theories.

6.2.2 Horizontal gene transfer

On a more personal note, one of my original goals laid out in my thesis proposal was to model evolutionary dynamics when considering both micro-evolutionary process of adaptive speciation and horizontal gene transfer (HGT). Since the application of large scale genomics has become feasible, there has been accumulating evidence that microbial genome evolution is highly affected, perhaps dominated, by HGT [41]. Multiple studies based on the phylogenetic conservation of microbial genes found that with a few exceptions metabolic genes (genes that code for enzymes able to catalyze a specific energy producing or carbon assimilatory pathway) are spread throughout the tree of life and decoupled from taxonomy [99–101, 106, 119], likely as a product of high levels of HGT. However, efforts to quantitatively describe both horizontal gene transfer and adaptive evolution are notably lacking.

To tackle this problem, I wrote a model based on the same modeling framework described in Chapters 2–4 but that also included the ability for individuals to go up or down in the dimensionality of their phenotype and to compete with individuals with a different dimension of phenotype. This fluidity in the dimension of trait space was added as a means to model the gain and loss of traits through homologous recombination. While I am proud of the model and still believe it worthy of further study, I quickly realized that the problem was too large and the dynamics too complicated, necessitating breaking the problem down into smaller pieces. The realization that epistatic interactions between traits are essential to create selective pressure on new combinations of phenotypes after a HGT event led to the investigation of adaptive evolution when considering an underlying rugged fitness landscape (Chapter 4). An observation that the same system can lead to differing cohorts of species depending only on the starting population and order of invasions led to an exploration of alternative evolutionary meta-stable states and Red Queen dynamics (Chapter 3). So, while this project remains uncompleted, it was both an important learning process for me and directly led to two other chapters and the completion of this thesis.
Bibliography


Matthias Zimmermann, Stéphane Escrig, Thomas Hübschmann, Mathias K. Kirf, Andreas Brand, R. Fredrik Inglis, Niculina Musat, Susann Müller, Anders Meibom, Martin Ackermann, and Frank Schreiber. Phenotypic heterogeneity in metabolic traits among single cells of a rare bacterial species in its natural environment quantified with a combination of flow cell sorting and nanosims. Frontiers in Microbiology, 06, April 2015.
Appendix A

Supplementary information for Chapter 2

A.1 Feasibility of random species

After randomly assembling a founding population we calculate the probability this initial random assortment of species is feasible. As we only consider Gaussian competition, any feasible community will also be globally stable [71]. The probability $N$ randomly selected, competitive species will be feasible always decreases with $N$. Additionally, the probability those $N$ species are feasible also always increases with the dimension of competition as the available niche space for those $N$ species is also greater.

When the probability of feasibility curves for each dimension are re-scaled to be a function of the community saturation ($H/ESS^d$) instead of diversity ($H$), the probability curves take on a remarkably similar shape regardless of dimension when viewed on a log-log scale [Fig. A.6] and it become clear that while the probability of feasibility for $N$ random species increases with dimension, the probability of feasibility for a random community of a given saturation actually decreases with increasing dimension. Notably, for $\sigma_\alpha = 0.6$ only in dimensions 1 and 2 were we able to randomly assemble a saturated, feasible community. In dimension 1, 34.77% of all 3 species communities (i.e., saturated) were feasible, and 9.54%, 0.44%, and 0.02% of communities with 4, 5, and 6 species (super-saturated) were found to be feasible respectively. In dimension 2, only 0.50% of 9 species communities (i.e., fully saturated) were feasible, and 0.08%, 0.06%, and 0.01% of 10-12 species (super-saturated) communities respectively were found to be feasible. While it is certainly possible to randomly select $N$ species that represent both a saturated or super-saturated and feasible community, in higher dimensions the probability of doing so is essentially zero [Fig. A.7].

A.1.1 Universal scaling of feasibility probability

The curves in Figures A.6 and A.8 corresponding to various dimensions looks similar to each other. Indeed, it turns out that for every $\sigma_\alpha$, and thus every unique ESS, there exists a scaling across dimensions that makes distributions of feasibility universal: The probability distribution of a randomly assembled community of a given saturation compared to the ESS being feasible scales as $a^{-d}$ [Fig. A.9]. The constant $a$ is non-universal and depends on $\sigma_\alpha$. This is because for each $\sigma_\alpha$ and thus for each ESS, there is a certain set of domains in
phenotype space where the species must be located for the community to be viable [Fig. 2.1]. The random assembly of species results in a given probability to have a viable community of a certain number of species for a given set of domains, that is, for a given $\sigma_\alpha$. The fraction of total phenotype space with dimension $d$ that corresponds to these domains scales as $a^{-d}$, which explains the observed scaling. Yet for a new $\sigma_\alpha$, such a set of domains changes in non-monotonic way due to the emergence of new species and resulting appearance, increase or shrinking of certain domains. Hence, the scaling factor is non-universal (in $\sigma_\alpha$) and even does not depend on $\sigma_\alpha$ in any systematic way.

A.2 Results of Statistical Test for Trait Dispersion in One Dimension

To test whether stable communities emerging through random assembly we used Welch’s $t$-test to compare top-down and bottom-up communities to Gaussian and uniformly distributed species of the same diversity as the communities. We also compared top-down and bottom-up communities to each other. We are using the coefficient of variation of the distance to the nearest neighbor in trait space ($CV_{NN}$) for each species as our metric for trait dispersion. Perfectly ordered communities (those that form a lattice in trait space) are maximally under dispersed compared to random and will have a $CV_{NN} = 0$. As communities become more dispersed in trait space they will have a larger $CV_{NN}$. As a metric of dispersion is meaningless in communities with 2 species, communities with diversity 3 through 6 (the maximal diversity for feasible communities with 1-dimensional competition and a $\sigma_\alpha = 0.6$) were tested.

Communities built through top-down and bottom-up assembly processes were not found to differ the the dispersion of their traits [Table A.1]. However, both types of randomly assembled community were found to be significantly ($\alpha < 0.05$) more regularly spaced in trait space compared to both methods of randomly distributed traits for all levels of diversity.

Because of computational limitations we did not statistically test the trait dispersion for communities with competition in greater than one dimension. However, graphically these communities have noticeably lower values $CV_{NN}$ compared both to both forms of randomly distributed traits of the same dimension, aligning with the statistical results from dimension one.

A.3 Supplementary figures
<table>
<thead>
<tr>
<th>Diversity</th>
<th>Model 1</th>
<th>Model 2</th>
<th>p value</th>
<th>Model 1 mean $CV_{NN}$</th>
<th>Model 2 mean $CV_{NN}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>Top Down</td>
<td>Bottom Up</td>
<td>0.178</td>
<td>0.337</td>
<td>0.191</td>
</tr>
<tr>
<td>4</td>
<td>Top Down</td>
<td>Bottom Up</td>
<td>0.866</td>
<td>0.443</td>
<td>0.432</td>
</tr>
<tr>
<td>5</td>
<td>Top Down</td>
<td>Bottom Up</td>
<td>0.253</td>
<td>0.614</td>
<td>0.560</td>
</tr>
<tr>
<td>6</td>
<td>Top Down</td>
<td>Bottom Up</td>
<td>0.427</td>
<td>0.572</td>
<td>0.621</td>
</tr>
<tr>
<td>3</td>
<td>Top Down</td>
<td>Gaussian Distributed</td>
<td>$3.14 \times 10^{-2}$ *</td>
<td>0.337</td>
<td>0.646</td>
</tr>
<tr>
<td>4</td>
<td>Top Down</td>
<td>Gaussian Distributed</td>
<td>$7.96 \times 10^{-5}$ **</td>
<td>0.443</td>
<td>0.814</td>
</tr>
<tr>
<td>5</td>
<td>Top Down</td>
<td>Gaussian Distributed</td>
<td>$1.88 \times 10^{-2}$ *</td>
<td>0.614</td>
<td>0.823</td>
</tr>
<tr>
<td>6</td>
<td>Top Down</td>
<td>Gaussian Distributed</td>
<td>$1.68 \times 10^{-4}$ **</td>
<td>0.572</td>
<td>0.923</td>
</tr>
<tr>
<td>3</td>
<td>Bottom Up</td>
<td>Gaussian Distributed</td>
<td>$7.09 \times 10^{-4}$ **</td>
<td>0.191</td>
<td>0.646</td>
</tr>
<tr>
<td>4</td>
<td>Bottom Up</td>
<td>Gaussian Distributed</td>
<td>$5.25 \times 10^{-5}$ **</td>
<td>0.432</td>
<td>0.814</td>
</tr>
<tr>
<td>5</td>
<td>Bottom Up</td>
<td>Gaussian Distributed</td>
<td>$3.96 \times 10^{-3}$ **</td>
<td>0.560</td>
<td>0.823</td>
</tr>
<tr>
<td>6</td>
<td>Bottom Up</td>
<td>Gaussian Distributed</td>
<td>$8.26 \times 10^{-4}$ **</td>
<td>0.621</td>
<td>0.923</td>
</tr>
<tr>
<td>3</td>
<td>Top Down</td>
<td>Uniformly Distributed</td>
<td>$9.66 \times 10^{-3}$ **</td>
<td>0.337</td>
<td>0.700</td>
</tr>
<tr>
<td>4</td>
<td>Top Down</td>
<td>Uniformly Distributed</td>
<td>$3.87 \times 10^{-3}$ **</td>
<td>0.443</td>
<td>0.696</td>
</tr>
<tr>
<td>5</td>
<td>Top Down</td>
<td>Uniformly Distributed</td>
<td>$3.88 \times 10^{-2}$ *</td>
<td>0.614</td>
<td>0.782</td>
</tr>
<tr>
<td>6</td>
<td>Top Down</td>
<td>Uniformly Distributed</td>
<td>$3.20 \times 10^{-4}$ **</td>
<td>0.572</td>
<td>1.04</td>
</tr>
<tr>
<td>3</td>
<td>Bottom Up</td>
<td>Uniformly Distributed</td>
<td>$8.81 \times 10^{-5}$ **</td>
<td>0.191</td>
<td>0.700</td>
</tr>
<tr>
<td>4</td>
<td>Bottom Up</td>
<td>Uniformly Distributed</td>
<td>$2.67 \times 10^{-3}$ **</td>
<td>0.432</td>
<td>0.696</td>
</tr>
<tr>
<td>5</td>
<td>Bottom Up</td>
<td>Uniformly Distributed</td>
<td>$7.05 \times 10^{-3}$ **</td>
<td>0.560</td>
<td>0.782</td>
</tr>
<tr>
<td>6</td>
<td>Bottom Up</td>
<td>Uniformly Distributed</td>
<td>$9.11 \times 10^{-4}$ **</td>
<td>0.621</td>
<td>1.04</td>
</tr>
</tbody>
</table>

Table A.1: **Statistical test for trait dispersion in one dimension.** To test for the dispersion of traits, we calculated the coefficient of variation of the nearest neighbor for each species in the communities ($CV_{NN}$). Communities randomly assembled through both top-down and bottom-up assembly processes were tested against random uniformly and Gaussian distributed traits as well as against each other using Welch’s t-test. One asterisks denotes significance with $\alpha < 0.05$ and two denotes significance for $\alpha < 0.01$. Please see Figure 2.6 for a graphical representation of the data tested.
Figure A.1: **ESS in dimension two and three.** Evolutionary stable states were calculated using adaptive dynamics. Panel A shows the ESS in 2D. Blue represents areas with negative invasion fitness. As the ESS is globally stable, no areas of positive invasion fitness exist. Panel B the ESS in 3D. $\sigma_\alpha = 0.6$

Figure A.2: **The final stable diversity of a randomly assembled community for $\sigma_\alpha = 0.5, 1.0$.** This is the same simulations as in Figure 2.3 but for $\sigma_\alpha = 1$ and 0.5 for panels A and B respectively. Communities were assembled with random species in 1-5 dimensions. Ecological dynamics were run for $10^8$ time steps. Hollow points represent communities that did not stabilize to a feasible community by the end of the simulation and still contain at least one species that will eventually go extinct. Grey lines are a regression using a nonlinear least squares fit to Michaelis-Menten dynamics ($y = \frac{ax}{b+x}$). Regressions were fit only to communities that have stabilized by the end of the simulation. The Michaelis-Menten curves are not mechanistic, and where not chosen to model the ecological dynamics in any way, but are asymptotic curves (asymptote equal to regression parameter $a$) that are a good visual fit for the data.
Figure A.3: **Final community saturation from randomly assembled species for** $\alpha = 0.5, 1.0$. This is the same simulations as in Figure 2.3 but for $\alpha = 1$ and 0.5 for panels A and B respectively. Communities were assembled with random species in 1-5 dimensions. Ecological dynamics were run for $10 \times 10^8$ time steps. Community saturation is measured as the diversity divided by the diversity of the ESS for the same ecosystem (for $\alpha = 0.5$, $H_{ESS} = 4^d$, for $\alpha = 1$, $H_{ESS} = 2^d$).

Figure A.4: **Community diversity and saturation as a function of the width of competition ($\alpha$).** Random communities of 100 species were assembled and ecological dynamics were run for $10^{12}$ time steps. As expected, as the width of competition ($\alpha$) increases (species are more generalist), the final diversity of the community decreases. However, the saturation of the communities peaks at an intermediate value of $\alpha$. This is because two communities with similar $\alpha$ will likely share the same diversity of their ESS, but the community with a larger $\alpha$ will have a smaller community on average when that community is assembled randomly. Colors represent communities competing in different numbers of dimensions. Hollow points represent communities that did not stabilize when the simulation concluded. Quartic carrying capacity function ($\alpha_K = 1$) and Gaussian competition kernel ($\alpha = 0.6$)
Figure A.5: **Example of community with transient dynamics.** An example of a community with transient dynamics. After $10^{12}$ time steps the community had not yet stabilized. Founding population contained 311 species with random phenotypes in 2-dimensional phenotype space. Panel A shows the final population configuration and the carrying capacity function (white = 1, darker means decreasing $K$). Panel B shows the population size of each species over the course of the simulation. The species that is undergoing transient extinction at the end of the simulation has a phenotype of $[-0.496, -0.935]$. Quartic carrying capacity and Gaussian competition function with $\sigma_\alpha = 0.6$. 
Figure A.6: **Probability randomly assembled communities of a given saturation are feasible.** Each color represents the dimension of the trait space (from 1 – 5). The grey line denotes the saturation point where the randomly assembled community has the same diversity as the ESS in that dimension. Each probability curve was generated by calculating the feasibility of $10^6$ communities with between 2 and 100 randomly chosen species for each dimension (2 to 50 for dimension 1). On average 10200 communities were simulated for each level of diversity in each dimension (double that for dimension 1), allowing us to calculate probabilities to the order of $10^{-4}$. Quartic carrying capacity function ($\sigma_K = 1$) and Gaussian competition kernel with $\sigma_\alpha = 0.6$. 
Figure A.7: Probability that randomly assembled communities of a given diversity are feasible as a function of the dimension. Each line (and color) represents communities of a given diversity. Curves were generated by calculating the feasibility of $\times 10^6$ communities with between 2 and 100 randomly chosen species (between 2 and 50 for 1D) for each dimension. On average 10200 communities (twice that for 1D) were simulated for each level of diversity in each dimension, allowing us to calculate probabilities to the order of $1 \times 10^{-4}$. Quartic carrying capacity function ($\sigma_K = 1$) and Gaussian competition kernel ($\sigma_\alpha = 0.6$)
Figure A.8: Probability randomly assembled communities of a given saturation compared to the ESS are feasible. This is the same simulations as in Figure A.6 but for $\sigma_\alpha = 1$ and 0.5 for panels A and B respectively. Each color represents the dimension of the trait space (from 1 – 5). The grey line denotes the saturation point where the randomly assembled community has the same diversity as the ESS in that dimension. Each probability curve was generated by calculating the feasibility of $10^6$ communities with between 2 and 100 randomly chosen species for each dimension (2 to 50 for dimension 1). On average 10200 communities were simulated for each level of diversity in each dimension (double that for dimension 1), allowing us to calculate probabilities to the order of $10^{-4}$. 
Figure A.9: **Universal scaling of probability that randomly assembled communities of a given saturation are feasible.** Each color represents the dimension of the trait space (from 1 – 5). The saturation of each community is multiplied by $2^d$ to illustrate the approximate universality of the curves. Just as in Figure 2.4, each probability curve was generated by calculating the feasibility of $10^6$ communities with between 2 and 100 randomly chosen species for each dimension (2 to 50 for dimension 1). On average 10200 communities were simulated for each level of diversity in each dimension (double that for dimension 1), allowing us to calculate probabilities to the order of $10^{-4}$. Quartic carrying capacity function ($\sigma_K = 1$) and Gaussian competition kernel with $\sigma_\alpha = 0.6$ were used.
Appendix B

Supplementary information for Chapter 3

B.1 Full Model Details.

We consider a general model of logistic growth and frequency-dependent competition based on a $d$-dimensional phenotype [39, 40]. For simplicity the model does not consider spatial interactions. Evolution is modeled in three ways: adaptive dynamics, an individual-based model, and partial differential equations.

B.1.1 Ecological Dynamics

Ecological dynamics follow logistic growth governed by a carrying capacity $K(\vec{x})$ and a competition function $\alpha(\vec{x}, \vec{y})$ where $\vec{x}$ and $\vec{y}$ are the phenotypes of competing types with $\vec{x}, \vec{y} \in \mathbb{R}^d$.

The competition function is defined such that $\alpha(\vec{x}, \vec{x}) = 1$, and for symmetric competition $\alpha(\vec{x}, \vec{y}) < 1$ for $\vec{x} \neq \vec{y}$. Thus, the Gaussian part of competition between types diminishes as their phenotypes becomes more distant and is maximal between individuals with the same phenotype. For symmetric competition the competition function is strictly Gaussian.

$$\alpha(\vec{x}, \vec{y}) = \exp \left( - \sum_{k=1}^{d} \frac{(x_k - y_k)^2}{2\sigma^2} \right) \quad (B.1)$$

For asymmetric competition, the competition function also includes an additional term.

$$\alpha(\vec{x}, \vec{y}) = \exp \left( \sum_{k,l=1}^{d} b_{kl}(x_k - y_l)x_l - \sum_{k=1}^{d} \frac{(x_k - y_k)^2}{2\sigma^2} \right) \quad (B.2)$$

This first term is the first order of Taylor expansion of a higher order, non-symmetric competition function and thus represents the simplest form of adding non-symmetric dynamics to the Gaussian function [39]. It includes the coefficients $b_{kl}$. For the non-symmetric competition simulations discussed here, a specific set of $b$ coefficients were chosen that resulted in periodic evolutionary dynamics [provided in Table B.4]. The models were also run with many other values for these coefficients, including a survey of randomly chosen values, but results were qualitatively similar to the values chosen. For a review of how these values
govern evolutionary dynamics in higher dimensions, please see Doebeli et al. \[40\].

The carrying capacity function \(K(\vec{x})\) represents the equilibrium population size of a population of only individuals with phenotype \(\vec{x}\). Two carrying capacity functions are discussed here. What is the quartic carrying capacity is defined as such.

\[
K(\vec{x}) = \exp \left( -\sum_{k=1}^{d} \frac{\vec{x}_k^4}{4} \right) \quad (B.3)
\]

The radially symmetric carrying capacity is as follows.

\[
K(\vec{x}) = \exp \left( -\frac{\left( \sum_{k=1}^{d} \vec{x}_k^2 \right)^2}{2} \right) \quad (B.4)
\]

Both functions are similar in that they are maximal at the origin and of the fourth order. This ensures that there is stabilizing selection toward \(\vec{x} = 0\) and that the phenotype space that is viable is bounded near the origin. The quartic carrying capacity function has an approximately square peak, while the radially symmetric function is circular [Fig. 3.1].

Together, ecological dynamics are as follows,

\[
\frac{dN_i}{dt} = rN_i(t) \left( 1 - \frac{\sum_{k=1}^{M} \alpha(\vec{x}_j, \vec{x}_i)N_j(t)}{K(\vec{x}_i)} \right) \quad (B.5)
\]

with \(N_i\) representing the population size of individuals with phenotype \(\vec{x}_i\), in a total population of \(M\) different phenotypes, and an intrinsic growth rate of \(r\).

**B.1.2 Adaptive Dynamics**

Using adaptive dynamics \[33, 36, 113\], the evolution of a phenotype \(\vec{x}\) can be described by a system of differential equations \(d\vec{x}/dt\). This is derived from the invasion fitness \(f(\vec{x}, \vec{y})\), which is the per capita growth rate of a rare mutant with phenotype \(\vec{y}\) in a resident population with phenotype \(\vec{x}\).

\[
f(\vec{x}, \vec{y}) = 1 - \frac{\alpha(\vec{x}, \vec{y})K(\vec{x})}{K(\vec{y})} \quad (B.6)
\]

This invasion fitness function relates how the growth rate of the resident is always decreased with the introduction of a new mutant unless \(\vec{x} = \vec{y}\) when \(f(\vec{x}, \vec{y}) = 0\). From this we can derive the selection gradient, \(s\), as the derivative of the invasion fitness with respect to the mutant, \(\vec{y}\), when it is equal to the resident, \(\vec{x}\).

\[
s_i(\vec{x}) = -\left. \frac{\partial\alpha(\vec{x}, \vec{y})}{\partial y_i} \right|_{y=x} + \frac{\partial K(\vec{x})}{\partial x_i} \frac{1}{K(\vec{x})} \quad (B.7)
\]
The adaptive dynamics are defined as

$$\frac{d\vec{x}}{dt} = \hat{M}(\vec{x})\vec{s}(\vec{x})$$  \hspace{1cm} (B.8)

where $\hat{M}$ is the mutation-covariance matrix describing the rate, size, and covariance of mutations in each phenotypic dimension. For simplicity we assume this is the identity matrix. Any formulation of this matrix with a positive diagonal would only change the speed of the evolution in the different dimensions, but would not change the characteristics of any evolutionary dynamics or stable states. The adaptive dynamics are therefore a set of differential equations that describe the evolutionary dynamics in $d$ dimensions for a given set of phenotypes.

Of note, while the Gaussian part of the competition kernel $\alpha$ affects whether diversification can occur and multi-species dynamics, because the selection gradient is evaluated at $\vec{y} = \vec{x}$, in the adaptive dynamics of monomorphic populations the Gaussian part of $\alpha$ disappears and we are left with just the effects of asymmetric competition. Because of the exponential nature of carrying capacity functions, the second term of the selections gradient, $\frac{\partial K(\vec{x})}{\partial x_i} \frac{1}{K(\vec{x})}$, reduces to just the partial derivative of the inner function with respect to the resident. For the quartic case the adaptive dynamics thus as follows

$$\frac{dx_k}{dt} = \sum_{l=1}^{d} b_{kl}x_l - x_k^3$$  \hspace{1cm} (B.9)

For the radially symmetric case the adaptive dynamics are

$$\frac{dx_k}{dt} = \sum_{l=1}^{d} \left( b_{kl}x_l - \frac{x_l^2}{2}\right)$$  \hspace{1cm} (B.10)

In order to include extinction and speciation events, an iterative algorithm is used: (1) solve for the ecological dynamics; (2) remove any newly extinct populations that fall below a minimum viable population size; (3) solve the adaptive dynamics for a given length of evolutionary time; (4) introduce a new mutant, with a phenotype a small, fixed distance from one of the resident populations or with a phenotype chosen from a Gaussian distribution with mean equal to the phenotype as one of the resident populations and a given variance $\sigma_{mut}^2$; (5) remove the mutant if it is not ecologically viable (invasion fitness of the mutant is negative); and (6) repeat the process until either an evolutionary stable state or a given amount of time is reached.

At given intervals, clusters are calculated using a hierarchical clustering algorithm such that any two population with phenotypes within a small distance, $z_{small}$, from each other are part of one cluster. Clusters are just an accounting device and do not affect dynamics. All parameters used can be found in Table [B.1].
B.1.3 Individual-Based Model

The individual-based model uses the same ecological dynamics as described above and simulated based on the Gillespie algorithm \cite{58}. Individual birth rates are assumed to be constant and equal to 1, while death rates, $\delta$, are frequency dependent and derived from the ecological dynamics.

\[
\delta_i = \sum_{j \neq i} \frac{\alpha(\vec{x}_j, \vec{x}_i)}{K(\vec{x}_i)K_{\text{max}}} \tag{B.11}
\]

Here the competition function, $\alpha$, and the carrying capacity function, $K$, are the same as in the adaptive dynamics, while $K_{\text{max}}$ is a constant that controls the height of the carrying capacity function to convert it from continuous to discrete populations. These rates are taken directly from the Lotka-Volterra equations, where the per capita growth rate of \[
1 - \frac{\sum_j \alpha(\vec{z}_j, \vec{z}_i)N_j(t)}{K(\vec{z}_i)}
\]

can be considered the birth rate minus the death rate. The individual-based model is thus a direct analog of the adaptive dynamics. For a larger discussion on the derivation of the individual-based dynamics of this model please refer to \cite{18, 32, 82}.

The simulation algorithm is as follows: (1) initiate the population with a randomly chosen initial population of a predetermined size; (2) update or calculate all individual death rates; (3) calculate the sum of all birth and death rates, $U = \sum_i (1 + \delta_i)$; (4) increment time by a random amount drawn from an exponential distribution with mean equal to $1/U$; (5) chose a random birth or death with probability equal to the ratio of the rate and the sum of all rates; (6) if a death rate is chosen, remove the chosen individual; if a birth rate is chosen, create a new individual with phenotype chosen from a Gaussian distribution with mean equal to the parent phenotype and variance $\sigma^2_{\text{mut}}$; (7) rerun steps 2-6 until the population is extinct or a specified time is reached.

Phenotypic clusters are calculated using a hierarchical clustering algorithm in which every individual in a cluster has a phenotype within a small distance of at least one other individual in the cluster. Individuals are added to a cluster at birth or a new cluster is created if the individual does not fit in any existing cluster. A cluster is updated when a member individual dies to see if the cluster splits. All parameters used can be found in Table \textbf{B.2}.

B.2 Numerical stability analysis.

While we were unable to analytically determine the stability of the communities that arose in our simulations, we were able to test for evolutionary metastability numerically. However, this method is computationally expensive, so we were only able to test for stability on a small number of representative simulations.

To test the stability the final population in a simulation we extensively sampled random
mutants around every resident in the community (250 mutants per resident). For each new mutant, we continued the adaptive dynamics simulation for a significant period of time (5% the length of the original simulation), while not allowing any other branching mutations to arise. We then checked whether the original residents and the mutant were all able to survive ($N_i > N_{small}$) and the mutant was able to diversify ($|\vec{z}_m - \vec{z}_i| > z_{small} \forall i$ for a mutant with phenotype $z_m$ and residents $z_i$) from the resident population. Any simulation in which no mutant can invade, coexist, and diversify is deemed an evolutionarily stable community.

While this method is unable to definitively prove stability as it is always possible that an extremely rare mutant could diversify or drive multiple residents extinct, we can at least demonstrate the metastability (as defined in the main text; any state that is maintained for a period significantly longer than its convergence) of these communities. An illustration of metastability can be seen in Figure B.1. Here, the convergence to the metastable cycle with 10 species takes approximately 25 evolutionary time units, after which the system resides in the metastable state until the end of the simulation, which lasts for another 975 time units. A clearer depiction of the early convergent dynamics can be seen in the main text in Figure 3.3.

**Figure B.1: Convergence to metastable limit cycle.** Here we define metastability operationally as any system that resides in a state much longer than it took to converge to it. Here, the system converges to a stable limit cycle in approximately 25 time steps and remains there for the duration of the simulation. The simulation were run using the radially symmetric carrying capacity and initiated with 18 random species. Panel A shows the complete history of evolutionary dynamics. Panel B is a depiction of the population at the end of the simulation. Colors in panel B represent the invasion fitness (per capita growth rate of a new mutant if it were to arise). Positive invasion fitness is shown in shades of orange (maximum of 0.091), negative in blue, and invasion fitness equal to zero in white. Arrows are proportional to the square root of the selection gradient for each species.

This numerical stability analysis was used to test each simulation illustrated in the main
text [Figs. 3.2 and 3.4]. Using the same small mutations as the original simulations, not a single mutant (of over 30,000 tested) was able to invade, coexist with, and differentiate from the original community. The same was true when we instead tested Gaussian mutations ($\sigma_{\text{mut}} = 0.05$). Only when we tested larger mutations (Gaussian mutations with $\sigma_{\text{mut}} = 0.1$) were 7 mutants (0.02% of those attempted) from two different simulations able to break the stability and diversify the community into a new, higher diversity state.

At least in the representative simulations tested, only large or extremely rare mutants are able to shift the community, proving that these states are indeed evolutionarily metastable.

Figures from the numerical stability analysis for each of these simulations can be found on-line at \url{https://www.zoology.ubc.ca/~rubin/AltEvoDiversity/}.

### B.3 PDE model.

In addition to the adaptive dynamics and individual-based models, we also ran partial differential equation simulations. PDEs represent the infinite population approximation of individual-based models \[18, 82\] and are useful for relaxing the phenotypes represented as a delta function and the separation of timescale between ecology and evolution assumptions of adaptive dynamics without the stochasticity of individual-based models.

The infinite population version of the individual based model gives the deterministic formulation of partial differential equations.

$$\frac{\partial N(\vec{x}, t)}{\partial t} = N(\vec{x}, t) \left( 1 - \frac{\int \alpha(\vec{x}, \vec{y}) N(\vec{y}, t) d\vec{y}}{K(\vec{x})} \right) + \delta_{\text{mut}} \sum_{k=1}^{d} \frac{\partial^2 N(\vec{x}, t)}{\partial x_k^2} \tag{B.12}$$

Here, $N(\vec{x}, t)$ is distribution of the population with phenotype $\vec{x}$ at time $t$ and $\delta_{\text{mut}}$ is diffusion coefficient that can be thought of as analogous to the rate of mutations and will not have qualitative effect on our simulations. The competition and carrying capacity functions are the same as described above. The PDE is numerically solved over a lattice. Because of memory limitations, using a high resolution lattice is infeasible, though we were able to run all 2-dimensional PDE simulations on a 200 x 200 lattice. This lattice is more than detailed enough to reveal any peaks and patterns that appear. The local maxima of the resulting distributions represent centers of clusters of individuals in the individual-based model.

Notably, like the individual-based model, the PDEs are not restricted to approximation of adaptive dynamics that phenotypes are represented as delta functions. Instead, the distributions produced by the PDEs “take up space” in the phenotype space. This can result in configurations with fewer local maxima than adaptive dynamics populations when run with the same parameters. Additionally, because the PDEs are a diffusion process, configurations cannot be trapped by small mutations. This makes the PDE simulations unsuited to studying the presence or absence of alternative stable configurations. They are however an useful comparison to the adaptive dynamics and individual-based models that
are fully deterministic and free of the assumptions intrinsic to adaptive dynamics.

When PDE simulations are run with symmetric competition, the resulting population densities are configured in the same 4x4 grid and two concentric circles as the comparable adaptive dynamics simulations [Figs. 3.2 and B.2]. The same concentric circles appear as ridges of high population density, but only the inner is peaked and far less distinctly than with the quartic grid. As the adaptive dynamics assumes species can be represented by a single phenotype without variance, continuous diversification around the circles is the only way for the population to mimic the circular ridge predicted by the PDE. This implies that with infinite population size (adaptive dynamics and PDE), simulations with symmetric competition and a radially symmetric carrying capacity eventually (though this process is slow) result in no distinct species or phenotypic clusters. However, as noted in the main text, this situation of continual diversification along concentric circles in trait space is likely a degenerate case that is cause by a radially symmetric carrying capacity function and Gaussian competition.

B.3.1 Within species phenotypic variation reduces diversity

For the asymmetric competition, PDE simulations with both quartic and radially symmetric carrying capacities result in similar, but less diverse patterns in comparison to the highest evolutionary stable diversity state from the adaptive dynamics simulations (10 versus 14 phenotypes for the quartic carrying capacity and 14 versus 16 phenotypes for the radially symmetric case) [Figs. 3.4 and B.2]. The reduced diversity is likely because the peaks in the adaptive dynamics are delta peaks, while those in the PDE have non-zero variance in phenotype space, restricting the number of distinct peaks. The radially symmetric carrying capacity simulation did exhibit the same clockwise rotation in both rings as displayed in the adaptive dynamics and individual-based models (video available on-line, Appendix B.5).

There has been previous theoretical work that predicts variation within species clusters has a negative effect on coexistence between competing species [66]. As species now occupy a distribution in trait space, rather than a single point, niche differentiation between species is reduced, impeding the maintenance of higher numbers of distinct phenotypes. As the PDE is the infinite population limit of the individual-based models, we would expect the same lower diversity at the global ESC when the individual-based simulations are run with very large communities and mutation sizes greater than some ϵ (these simulations were computationally infeasible to run). While we don’t expect the other results (the presence of locally stable ESSs or limit cycles) from this paper to be affected by the lower diversity, we feel it is a salient point worth considering when comparing theoretical models of diversification to expectations for natural populations.

All parameters used can be found in Table B.3.
Figure B.2: The final population density when simulated using a PDE. Higher densities are darker and lower densities are lighter. Contour lines are shown in blue. 3-dimensional, interactive versions of the same figures and videos of the dynamics are available online [Table B.3]. Population distributions generated using the PDE models result in similar configurations to those emergent from the Adaptive Dynamics, but with fewer distinct species resulting from intra-species phenotypic variance. The asymmetric competition and radially symmetric carrying capacity simulation exhibits the same clockwise rotation displayed in the adaptive dynamics and individual-based simulations.
Table B.1: Parameters and variables used to generate adaptive dynamics data and figures.

### B.4 Parameters

*Evolutionary velocity is defined as the population weighted average magnitude of the rates of the phenotype vectors:

\[
v = \sum_{i=1}^{M} \frac{N_i \sum_{k=1}^{d} |dx_{ik}/dt|}{\sum_{j=1}^{M} N_j}
\]  

(B.13)

After each step solving the adaptive dynamics (step 3 as outlined above), the evolutionary velocity is checked, and if \(v < v_{\text{min}}\), the simulation is deemed stable and stopped.

Table B.2: Parameters and variables used to generate individual-based model data and figures.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\sigma_\alpha)</td>
<td>0.5</td>
<td>Standard deviation of the competition kernel</td>
</tr>
<tr>
<td>(r)</td>
<td>1.1</td>
<td>The intrinsic growth rate</td>
</tr>
<tr>
<td>(\sigma_{\text{mut}})</td>
<td>0.005</td>
<td>Standard deviation of mutation</td>
</tr>
<tr>
<td>(T_{\text{max}})</td>
<td>(10^5)</td>
<td>Number of time steps simulations run for</td>
</tr>
<tr>
<td>(K_{\text{max}})</td>
<td>400</td>
<td>The height of the carrying capacity function at the origin</td>
</tr>
<tr>
<td>(\delta_{\text{cluster}})</td>
<td>(50\sigma_{\text{mut}})</td>
<td>The maximum distance between individuals of the same cluster</td>
</tr>
</tbody>
</table>

Table B.3: Parameters and variables used to generate partial differential equation model data and figures.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\sigma_\alpha)</td>
<td>0.5</td>
<td>Standard deviation of the competition kernel</td>
</tr>
<tr>
<td>(N_{\text{bins}})</td>
<td>200</td>
<td>The number of bins in each dimension</td>
</tr>
<tr>
<td>(z_{\text{range}})</td>
<td>((-2, 2))</td>
<td>The minimum and maximum phenotype in each dimension</td>
</tr>
<tr>
<td>(\delta_{\text{mut}})</td>
<td>0.01</td>
<td>The amplitude of diffusion modeling mutation</td>
</tr>
<tr>
<td>(T_{\text{max}})</td>
<td>(10^3)</td>
<td>Number of time steps simulations run for</td>
</tr>
<tr>
<td>(\sigma_N)</td>
<td>0.1</td>
<td>Standard deviation of the initial spread around the origin</td>
</tr>
<tr>
<td>(\delta_t)</td>
<td>2</td>
<td>The integration time step</td>
</tr>
</tbody>
</table>
Table B.4: Default asymmetric competition parameters. The default values of parameter $b$ that dictates the competition asymmetry used in all asymmetric competition simulations.

$$
\begin{bmatrix}
0.40716468083977814 & -0.60799602828722576 \\
0.94740291877661453 & 0.65155997501420926
\end{bmatrix}
$$

B.5 Videos, additional figures, and model source code.

Videos of the evolutionary dynamics for all simulations highlighted in the paper (including adaptive dynamics, individual-based, partial differential equation, and stability analysis simulations) can be found on-line at [https://www.zoology.ubc.ca/~rubin/AltEvoDiversity/](https://www.zoology.ubc.ca/~rubin/AltEvoDiversity/). Additional figures including 3-dimensional, interactive landscapes of the final population density of PDE simulations can be found here as well. Source code for the model is also included.
Appendix C

Supplementary information for Chapter 4

C.1 Supplementary figures

Figure C.1: The number of peaks in the carrying capacity landscape. Three parameters used to generate the random ruggedness, the number of Gaussian curves that are laid out at equal intervals between -2 and 2 ($m$), the width of each Gaussian ($\sigma^2_R \in \mathbb{R}_{\geq 0}$), and the amplitude of the lowest valley in the randomly generated ruggedness ($A_R \in [0,1]$). The number of peaks in the rugged carrying capacity function is relatively indifferent to the number of Gaussian curves used in the generation function ($m$). A local peak were determined numerically by breaking the rugged landscape into 1000 sequential bins and defined as any bin with a larger carrying capacity than both of it’s neighbors. For panel A $\sigma^2_R$ was set to 0.02 and $A_R$ to 0.01, 0.05, 0.1, 0.25, or 0.5. For panel B $A_R$ was set to 0.1 and $\sigma^2_R$ to 0.005, 0.01, 0.025, or 0.05. The number of Gaussians used in the algorithm, $m$, was then chosen randomly between 3 and 1000. Curves represent the running mean with Gaussian weighting and shading the 95% confidence interval of that running mean. 50 landscapes with different values of $m$ were used to generate each curve. The global carrying capacity is a quartic function and the strength of competition, $\sigma_\alpha = 0.6$. 
Figure C.2: Proportion of phenotype space with positive invasion fitness after ecological saturation. Histogram of the proportion of the phenotype space with positive invasion fitness at the end of the simulation. The ecological simulations starting with a saturated population are shown in panel A and the evolutionary simulations starting with a single species in panel B. Note the x-axis for panel A goes from 0 to 0.06, while the x-axis for panel B is from 0 to 1. Evolutionary simulations with a proportion of invasion fitness equal to 0 represent populations at the ESS. Evolutionary simulations with a very large proportion of the phenotype space open to invasion are due to local ruggedness restricting diversification and evolution in phenotype space.
Figure C.3: Examples pairwise invasion diagrams for rugged carrying capacity landscapes. Pairwise invasion diagrams for the same landscapes included in Figure 4.1. The x-axis represents the resident phenotype and y-axis the mutant phenotype. The black areas indicate mutants that have a positive growth rate when introduced to a monomorphic population of the resident. If assuming small mutations, the $y = x$ line is indicative of the evolutionary dynamics. If there is black above and white below $y = x$, selective pressure will push the population to evolve to a larger phenotype and vice-versa. Places where the area of positive invasion fitness crosses the diagonal indicate peaks and valleys in the landscape.
Figure C.4: Examples of rugged carrying capacity landscapes with final population after evolution starting from founding species. Each rugged carrying capacity landscape is shown in blue, the baseline smooth carrying capacity kernel in grey, the initial population as a large hollow, red point, and the population after evolution as solid, red points. Rows denote the amplitude of the local ruggedness ($A_R$ between 1% and 50%) and columns denote the period of the local ruggedness ($\sigma^2_R = 0.005$ to $\sigma^2_R = 0.05$). Local ruggedness is generated by adding together 250 Gaussian distributions that are laid out on an equal interval between $-2$ and 2, with the width defined by $\sigma^2_R$ and heights randomly chosen from a Gaussian distribution with $\mu = 1$, $\sigma = 1$. The generated local ruggedness is then re-scaled such that the minimum is equal to the amplitude and then multiplied by the global landscape kernel ($K(x) = \exp(-x^4/4)$). Thus, an amplitude $A_R = 0$ results in no ruggedness while $A_R = 1$ means that the lowest valley in the landscape will have a carrying capacity equal to 0. An amplitude $A_R = 0.5$ means that the lowest valley in the landscape has a carrying capacity equal to half what it would be with a purely smooth carrying capacity function. A single species was randomly selected ($x \sim [-2, 2]$) as the initial species. Evolution was then simulated through a trait substitution process until 500 consecutive mutants were unable to invade. For pairwise invasion diagrams of the same landscapes please see Fig. C.3.
Appendix D

Supplementary information for Chapter 5

D.1 Trait spaces

As there is a one-to-one map, \((\alpha, \beta) \mapsto (\bar{z}, \sigma^2_z)\), in addition to using \(\alpha\) and \(\beta\), a Beta distribution can also be defined in terms of its mean \((\bar{z})\) and variance \((\sigma^2_z)\) such that

\[
\begin{align*}
\bar{z} &= \frac{\alpha}{\alpha + \beta}, \quad \sigma^2_z = \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)} \quad \text{if} \quad \bar{z} \in (0, 1), \quad \sigma^2_z \in (0, \bar{z} - \bar{z}^2) \\
\end{align*}
\]

(D.1)

Additionally, we define the relative variance, \(v\), to be the variance scaled by the maximum possible variance for the mean \(\bar{z}\), so that \(\sigma^2_z \in (0, \bar{z} - \bar{z}^2) \mapsto v \in (0, 1)\).

\[
\begin{align*}
\bar{z} &= \frac{\alpha}{\alpha + \beta}, \quad v = \frac{\sigma^2_z}{\bar{z} - \bar{z}^2} = \frac{1}{\alpha + \beta + 1} \quad \text{if} \quad \bar{z}, v \in (0, 1) \\
\end{align*}
\]

(D.2)

As this is also an one-to-one function, the beta distribution can also be defined by a mean and relative variance.

The \(\alpha, \beta\) trait space is defined on \(\alpha, \beta \in (0, \infty)\) [Fig. D.1a] and the \(\bar{z}, \sigma^2_z\) trait space is defined on \(\bar{z} \in (0, 1), \quad \sigma^2_z \in (0, \bar{z} - \bar{z}^2)\) [Fig. D.1b]. For populations in the \(\alpha, \beta\) trait space, small changes in one of the two parameters (i.e., mutation) can have disproportionate effects on the shape of the distribution depending on where the distribution is in the trait space. For instance, a mutation of \(\alpha 0.1\) to \(0.2\) is going to have a much larger effect on the phenotype distribution than from \(100.1\) to \(100.2\). Additionally, distributions defined by a mean \((\bar{z})\) and spread metric \((\sigma^2_z\) or \(v\)) are more biologically intuitive as they are easier to provide a mechanistic motivation. For instance, \(\bar{z}\) and \(\sigma^2_z/v\) can be loosely interpreted as the preference for one resource over the other and the level of phenotypic heterogeneity in the population, respectively. In contrast, it is hard to imagine a biological interpretation of \(\alpha\) and \(\beta\). Given the mathematical convenience of dealing with a trait space defined on \([0, 1]\) we will focus on evolution in the \(\bar{z}, v\) trait space.
Figure D.1: **Trait spaces.** Shown are the areas in the trait spaces that correspond to the different shapes of the phenotypic Beta distribution. White areas are not defined in the given trait space. The lightest shade of grey represents monomorphic beta distributions with a peak located $\in (0, 1)$ [Fig. 5.3a]. The darkest shade of grey represents dimorphic beta distributions with peaks at 0 and 1 [Fig. 5.3c]. The intermediate shade of grey represents monomorphic phenotype distributions with the peak located at 0 or 1 [Fig. 5.3b]. The point $\bar{z} = \frac{1}{2}, \frac{1}{3}$ ($\sigma^2_z = \frac{1}{12}$ or $\alpha, \beta = 1$) represents a uniform distribution. Note, the $\alpha, \beta$ trait space is defined on $(0, \infty)$. The other two trait spaces are finite.

**D.2 Complete equations**

The full population and resource dynamics are described by:

$$\frac{dN}{dt} = (1 - c_v v) \sum_i N_i \left( \bar{z}_i \ast \frac{r_A[A]}{K_A + [A]} Y_A + \int_0^1 g(z) f(z; \alpha_i, \beta_i) dz \ast \frac{r_B[B]}{K_B + [B]} Y_B - \lambda \right)$$  \hfill (D.3)

$$\frac{d[A]}{dt} = (1 - c_v v) \sum_i -N_i \left( \bar{z}_i \ast \frac{r_A[A]}{K_A + [A]} \right) + \gamma_A \left( \omega_A \sin \left( \frac{2\pi}{T_A} \right) + 1 \right)$$  \hfill (D.4)

$$\frac{d[B]}{dt} = (1 - c_v v) \sum_i N_i \left( Y_{cf} \ast \bar{z}_i \ast \frac{r_A[A]}{K_A + [A]} - \int_0^1 g(z) f(z; \alpha_i, \beta_i) dz \ast \frac{r_B[B]}{K_B + [B]} \right) + \gamma_B \left( \omega_B \sin \left( \frac{2\pi}{T_B} \right) + 1 \right)$$  \hfill (D.5)

$$f(z; \alpha_i, \beta_i) = \frac{1}{\Omega(\alpha_i, \beta_i)} z^{\alpha_i - 1}(1 - z)^{\beta_i - 1}$$  \hfill (D.6)

$$\Omega(\alpha_i, \beta_i) = \int_0^1 u^{\alpha_i - 1}(1 - u)^{\beta_i - 1} du$$  \hfill (D.7)

$$\left\{ \alpha_i = \bar{z}_i \left( \frac{1}{v_i} - 1 \right), \beta_i = \frac{(v_i - 1)(\bar{z}_i - 1)}{v_i} \right\} \bar{z}_i, v_i \in (0, 1)$$  \hfill (D.8)
The state variables $[A]$ and $[B]$ represent the resource concentrations and $N$ represents the total population abundance. $N_i$ represents the abundance of genotype $i$ (as defined by the parameters $\bar{z}_i$ and $v$), such that $N = \sum_i N_i$.

Total population growth is modelled as the consumption of resources $A$ and $B$ based on Michaelis-Menten kinetics (with a maximum rate of consumption $r_X$, Michaelis-Menten constant $K_X$, and growth yield per unit resource consumed $Y_X$ for each resource $X$) and a constant death rate ($\lambda$) $[\text{Equation D.3}]$. The phenotypic distribution of the relative consumption of each resource for genotype $i$ is defined by the probability density function of the beta distribution with a given mean ($\bar{z}_i$) and relative variance ($v_i$) $[\text{Equations D.6-D.8}]$. Population growth decreases linearly with increased relative variance ($v$) at a rate $c_v$, representing a cost to high variance.

Resource dynamics are described as periodic resource influx (with mean $\gamma_X$, period $T_X$, and amplitude $\omega_X$ for each resource $X$) minus the resources consumed $[\text{Equations D.4-D.5}]$. Additionally, resource $B$ is created due to cross feeding at a rate of $Y_{cf}$ per unit $A$ consumed.

When there is no cost to heterogeneity, cross-feeding, or resource fluctuations ($c_v = Y_{cf} = \omega_A = \omega_B = 0$), the base model is recovered $[\text{Equations 5.8-5.11}]$. 

D.3 Supplementary figures

Figure D.2: **Pairwise invasibility.** Black indicates regions where the mutant can invade ($\dot{N}_{mut} > 0 \mid A^*, B^*$), white are regions where the mutant cannot invade ($\dot{N}_{mut} < 0 \mid A^*, B^*$), and grey are regions where the mutant’s growth is identical to that of the parent ($\dot{N}_{mut} = 0 \mid A^*, B^*$). The equilibrium environment of the parental strain ($A^*, B^*$) was solved numerically, resulting in the noise when $\dot{N}_{mut}$ is very close to 0. [$r_A = 1.1, r_B = 1.01, Y_A = 0.8, Y_B = 0.5, \lambda = 0.01, \gamma_A = \gamma_B = 1.0, k_A = k_B = 1.0, c = 0.3, \bar{z} = 0.5, v = 0.1$]
Figure D.3: **Selection gradients for other values of $c$.** Each plot is a visualization of the deterministic evolution in two dimensions for different constraint values. The $\frac{d\bar{z}}{dt}$ nullclines are shown in blue. As there are no singular points in the one-dimensional $v$ selection gradient, there are no $\frac{dv}{dt}$ nullclines. Solid nullclines are evolutionarily stable in that dimension. Dashed nullclines are convergent stable but evolutionarily unstable. Dotted nullclines are unstable. $[r_A = 1.1, r_B = 1.01, Y_A = 0.8, Y_B = 0.5, \lambda = 0.01, \gamma_A = \gamma_B = 1.0, k_A = k_B = 1.0]$
Figure D.4: **Pairwise invasibility when considering a cost the heterogeneity.** Black indicates regions where the mutant can invade ($\dot{N}_{mut} > 0 \mid A^*, B^*$), white are regions where the mutant cannot invade ($\dot{N}_{mut} < 0 \mid A^*, B^*$), and grey are regions where the mutant’s growth is identical to that of the parent ($\dot{N}_{mut} = 0 \mid A^*, B^*$). The equilibrium environment of the parental strain ($A^*, B^*$) was solved numerically, resulting in the noise when $\dot{N}_{mut}$ is very close to 0. 

$[r_A = 1.1, r_B = 1.01, Y_A = 0.8, Y_B = 0.5, \lambda = 0.01, \gamma_A = \gamma_B = 1.0, k_A = k_B = 1.0, c = 0.3, \bar{z} = 0.5]$
Figure D.5: **Additional evolutionary trajectories.** Two more examples of the simulated trajectories of $\bar{z}$ and $v$ showing a branching “false-start” and a population that is both genetically dimorphic and phenotypically heterogeneous. Blue represents the genetic values of $\bar{z}$ and red represents the values of $v$. The size of the dots indicates the relative population size of that genotype. The y-axis is time measured by the number of mutations. Because we show both variables on the same axis, we are showing a 2-dimensional projection of the 3-dimensional space. All simulations are run with the same parameterization and run until evolutionary equilibrium, which is defined as 30 consecutive unsuccessful mutations.

$[r_A = 1.1, r_B = 1.01, Y_A = 0.8, Y_B = 0.5, \lambda = 0.01, \gamma_A = \gamma_B = 1.0, k_A = k_B = 1.0, c = 0.3, \bar{z} = 0.3, v = 0.1, \mu_{mut} = 1^{-5}, \sigma_{\bar{z}}^2 = \sigma_v^2 = 0.02]$
Figure D.6: **Probability of phenotypic heterogeneity under cross feeding.** In Panel A, trajectories that result in a genetically dimorphic population for $\bar{z}$ are shown as solid lines for parallel and hierarchical (cross feeding) resource pathways. Dashed lines indicate the probability of branching false-starts. In Panel B, trajectories that result in a genetically dimorphic population for $\bar{z}$ are shown in blue, phenotypic heterogeneous populations in blue, mixed phenotypic heterogeneity and genetic dimorphic populations in pruple, and monomorphic, non-heterogeneous populations in green. \([r_A = 1.1, r_B = 1.01, Y_A = 0.8, Y_B = 0.5, \lambda = 0.01, \gamma_A = \gamma_B = 1.0, k_A = k_B = 1.0, c = 0.3, \bar{z} = 0.3, v = 0.1, \mu_{mut} = 1^{-5}, \sigma_v^2 = \sigma_{\bar{z}}^2 = 0.015, Y_{cf} = 1.0]\)

Figure D.7: **Probability of phenotypic heterogeneity given a cost to heterogeneity.** Trajectories that result in a genetically dimorphic population for $\bar{z}$ are shown as a solid line. The dashed lines indicates the probability of branching false-starts. The dotted line represents the approximate emergence of the singular point for $v$. \([r_A = 1.1, r_B = 1.01, Y_A = 0.8, Y_B = 0.5, \lambda = 0.01, \gamma_A = \gamma_B = 1.0, k_A = k_B = 1.0, c = 0.3, \bar{z} = 0.3, v = 0.1, \mu_{mut} = 1^{-5}, \sigma_v^2 = \sigma_{\bar{z}}^2 = 0.015]\)